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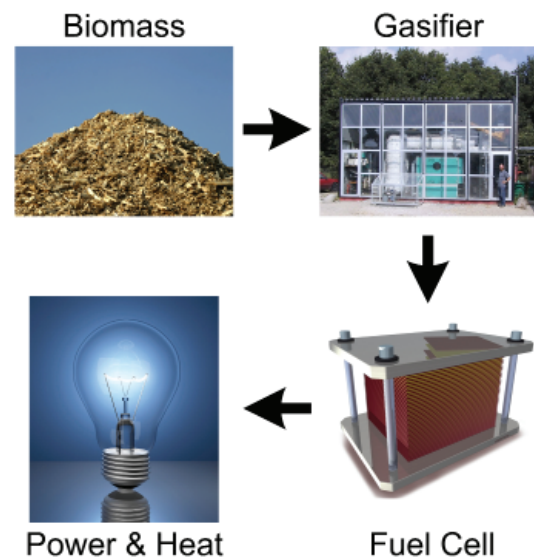
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Design and Optimization of an Integrated Biomass Gasification and Solid Oxide Fuel Cell System

PhD Thesis



Christian Bang-Møller
DCAMM Special Report no. S112
April 2010

DESIGN AND OPTIMIZATION OF AN INTEGRATED BIOMASS GASIFICATION AND SOLID OXIDE FUEL CELL SYSTEM

By

Christian Bang-Møller

A thesis submitted in partial fulfilment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

at the

TECHNICAL UNIVERSITY OF DENMARK

2010

Christian Bang-Møller

**DESIGN AND OPTIMIZATION OF AN INTEGRATED BIOMASS
GASIFICATION AND SOLID OXIDE FUEL CELL SYSTEM**

Technical University of Denmark
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Section of Thermal Energy Systems
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PREFACE

This thesis is submitted as a partial fulfilment of the requirements for the Ph.D. degree at the Technical University of Denmark.

The three year study was carried out at the Department of Mechanical Engineering, Section of Thermal Energy Systems from February 2007 to April 2010 under the supervision of Associate Professor Masoud Rokni and co-supervision of Associate Professor and Head of Section Brian Elmegaard and Associate Professor Ulrik Birk Henriksen.

An external research stay was conducted from August 2008 to November 2008 in Golden, Colorado, USA, at Colorado School of Mines (CSM) and the National Renewable Energy Laboratory (NREL), a research facility under the U.S. Department of Energy. Supervisors at CSM were Assistant Professor Robert Braun, Division of Engineering, and Professor Anthony M. Dean, Chemical Engineering Department.

The Ph.D. study was funded by the Technical University of Denmark and included membership of two research schools: DCAMM (Danish Center for Applied Mathematics and Mechanics) and HyFC (Hydrogen and Fuel Cell Academy).

The thesis is written as a monograph, but a number of papers have been published based on the work in this research study (see List of Publications on page IX).



Christian Bang-Møller
Kgs. Lyngby, April 2010

ABSTRACT

Development of sustainable power plants has gained focus in the recent years and utilization of biomass resources are seen as a pathway towards a sustainable combined heat and power (CHP) production. Biomass resources are distributed, thus decentralized biomass conversion would avoid extensive cost for biomass transportation. Traditional decentralized CHP plants suffer from low net electrical efficiencies compared to central power stations, though. Especially small-scale and dedicated biomass CHP plants have poor electrical power yield. Improving the electrical power yield from small-scale CHP plants based on biomass will improve the competitiveness of decentralized CHP production from biomass as well as move the development towards a more sustainable CHP production.

The aim of this research is to contribute to enhanced electrical efficiencies and sustainability in future decentralized CHP plants. The work deals with the coupling of thermal biomass gasification and solid oxide fuel cells (SOFCs), and specific focus is kept on exploring the potential performance of hybrid CHP systems based on the novel two-stage gasification concept and SOFCs. The two-stage gasification concept is developed and demonstrated at the Technical University of Denmark and performs with a high cold gas efficiency, 93% (LHV), and a clean product gas suitable for electrochemical conversion in SOFCs.

A zero-dimensional component model of an SOFC, including an electrochemical model, is developed and calibrated against published data from Topsoe Fuel Cells A/S. The SOFC component model predicts the SOFC performance at various operating conditions and is suited for implementation in system-level models using the simulation software DNA. Furthermore, it is used for issuing guidelines for optimal SOFC operation.

A system-level modelling study of three conceptual plant designs based on two-stage gasification of wood chips with a thermal biomass input of ~ 0.5

MW_{th} (LHV) is presented. Product gas is converted in a micro gas turbine (MGT) in the first plant design, in SOFCs in the second, and in a combined SOFC-MGT arrangement in the third. The plant scenarios are investigated by system-level modelling combining zero-dimensional component models including the developed SOFC component model. The SOFCs convert the product gas more efficiently than the MGT, which is reflected by the net electrical efficiency of the gasifier and MGT system in opposition to the gasifier and SOFC configuration – $\eta_{\text{el}}=27\%$ versus $\eta_{\text{el}}=43\%$ (LHV). By combining SOFCs and a MGT, the SOFC off gases are utilized in the MGT to generate additional power and the SOFCs are pressurized, which improves the efficiency to as much as $\eta_{\text{el}}=55\%$ (LHV). Variation of the different operating conditions reveals an optimum for the chosen pressure ratio with respect to the resulting electrical efficiency. Furthermore, the SOFC operating temperature and fuel utilization should be maintained at a high level and the cathode temperature gradient maximized.

Based on 1st and 2nd law analyses, the plant layout of the SOFC-MGT scenario is optimized obtaining a net electrical efficiency of $\eta_{\text{el}}=58\%$ (LHV). The performance gain is mainly ensured by an improved heat exchanger network. The optimization effort only required the installation of one additional component, an extra product gas preheater, ensuring reduced exergy destructions in several components and an increased TIT, thus boosting the MGT power output.

RESUMÉ (DANISH SUMMARY)

Opmærksomhed på udvikling af bæredygtige kraftværker er forøget de senere år, og udnyttelse af biomasseressourcer ses som en vej mod bæredygtig kraftvarmeproduktion. Biomasseressourcer dyrkes spredt, hvorved omsætning af disse biomasseressourcer i decentrale anlæg vil kunne reducere omkostninger forbundet med transport af biomassen. Dog lider traditionelle decentrale kraftvarmeværker under lav el-virkningsgrad sammenlignet med centrale værker. Specielt små og dedikerede biomassekraftvarmeværker har lavt el-udbytte. Forøget el-udbytte i decentrale biomassekraftvarmeværker vil forbedre konkurrenceevnen for små biomassekraftvarmeværker og skubbe udviklingen mod en mere bæredygtig kraftvarmeproduktion.

Formålet med denne forskning er at bidrage til forhøjede el-virkningsgrader og bæredygtighed i fremtidige decentrale kraftvarmeværker. Studiet omhandler sammenkoblingen af termisk biomasseforgasning og fastoxidbrændselsceller (Solid Oxide Fuel Cells, SOFCs) med fokus på vurdering af potentialet i kraftvarmeanlæg baseret på den udviklede tottrinsforgasningsproces og SOFC-brændselsceller. Tottrinsforgasningsprocessen er udviklet og demonstreret på Danmarks Tekniske Universitet, og processen opnår en høj koldgasvirkningsgrad, 93 % baseret på nedre brændværdi (LHV), og producerer en ren forgasningsgas, som er anvendelig til elektrokemisk omsætning i SOFC-brændselsceller.

En nuldimensionel komponentmodel af en SOFC, inklusiv en elektrokemisk model, er udviklet og kalibreret mod publicerede data fra Topsoe Fuel Cells A/S. SOFC-komponentmodellen beregner el-virkningsgraden af brændselscellerne afhængig af operationsbetingelser, og modellen er velegnet til brug i systemmodellering ved brug af simuleringsværktøjet DNA. Ydermere anvendes SOFC-komponentmodellen til at stikke retningslinjer for optimal drift af brændselscellerne.

Et systemmodelleringsstudie udføres for tre konceptuelle anlægsdesign baseret på tottrinsforgasning af træflis med et termisk biomasse input på ~ 0.5 MW_{th} (LHV). Forgasningsgassen omsættes i en mikrogasturbine (MGT) i det første anlægsdesign, i SOFC-brændselsceller i det andet og i et kombineret SOFC-MGT system i det tredje. De tre anlægsdesign er analyseret ved hjælp af systemmodellering ved at sammensætte nuldimensionelle komponentmodeller, inklusiv den udviklede SOFC-komponentmodel. Brændselscellerne omsætter forgasningsgassen mere effektivt end mikrogasturbinen, hvilket ses i el-virkningsgraderne for forgasser og MGT-systemet samt forgasser og SOFC-systemet – $\eta_{el}=27\%$ mod $\eta_{el}=43\%$ (LHV). Ved at kombinere brændselsceller og mikrogasturbine udnyttes udstødningsgasserne fra brændselscellerne til yderligere el-produktion, og brændselscellerne tryksættes, hvilket resulterer i en væsentligt højere el-virkningsgrad på $\eta_{el}=55\%$ (LHV). Parametervariation af de forskellige operationsbetingelser viser, at trykforholdet har et optimum i forhold til den resulterende el-virkningsgrad. Ydermere bør brændselscellernes operationstemperatur og brændselsomsætningsgrad fastholdes på et højt leje, og katodetemperaturgradienten bør maksimeres.

Baseret på energi- og exergianalyser optimeres systemdesignet af SOFC-MGT scenariet så det opnår en el-virkningsgrad på $\eta_{el}=58\%$ (LHV). Den højere el-virkningsgrad skyldes hovedsageligt et forbedret varmevekslernetværk. Optimeringen kræver kun installation af én komponent yderligere, en ekstra forgasningsgasforvarmer, som reducerer exergidestruktionen i flere komponenter samt forøger turbineindløbstemperaturen, hvorved mikrogasturbinens el-udbytte forøges.

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LIST OF PUBLICATIONS

The work in this PhD study has led to several publications in different formats. Below is listed the publications of significance. The papers can be found in the Appendix G, Appendix H, and Appendix I.

I. ISI Journal Paper

Bang-Møller C., Rokni M. Thermodynamic Performance Study of Biomass Gasification, Solid Oxide Fuel Cell and Micro Gas Turbine Hybrid Systems. *Energy Conversion and Management*. 2010, vol. 51, issue 11, pp. 2330-2339. doi:10.1016/j.enconman.2010.04.006.

II. Proceedings Paper - Peer Reviewed Manuscript

Bang-Møller C., Rokni M. Modelling a Combined Heat and Power Plant based on Gasification, Micro Gas Turbine and Solid Oxide Fuel Cells. In: Elmegaard B., Veje C., Nielsen M.P., Mølbak T. (eds.), *Proceedings of SIMS 50: Modelling of Energy Technology*. ISBN 978-87-89502-88-5. The Technical University of Denmark. Fredericia, Denmark. 2009, pp. 189-196.

III. Proceedings Paper - Peer Reviewed Abstract

Bang-Møller C., Rokni M. Modelling of a Biomass Gasification Plant Feeding a Hybrid Solid Oxide Fuel Cell and Micro Gas Turbine System. In: Sønderberg P.L., Larsen H.H. (eds.), *Proceedings of Risø International Energy Conference 2009: Energy solutions for CO₂ emission peak and subsequent decline*. ISBN 978-87-550-3783-0. Risø National Laboratory for Sustainable Energy. Roskilde, Denmark. 2009, pp. 289-299.

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NOMENCLATURE

Roman Symbols

A_{ij}	number of atoms of element j in each molecule of compound i [-]
ASR	area specific resistance [$\Omega \text{ cm}^2$]
CC	carbon conversion factor [-]
E	reversible open circuit voltage [V]
E_{act}	activation energy [J mol^{-1}]
F	Faradays constant [C mol^{-1}]
\dot{G}	Gibbs free energy [J s^{-1}]
g_{f}	Gibbs free energy [J mol^{-1}]
h	enthalpy [kJ kg^{-1}]
h_{f}	enthalpy of formation [J mol^{-1}]
i	current density [mA cm^{-2}]
i_{as}	anode limiting current density [mA cm^{-2}]
i_{n}	internal current density [mA cm^{-2}]
i_0	exchange current density [mA cm^{-2}]
k	total number of chemical compounds leaving the system [-]
LHV	lower heating value [kJ kg^{-1}]
\dot{m}	mass flow [kg s^{-1}]
$METH$	fraction of non-equilibrium methane [vol-%]
N	total number of chemical elements in the system [-]
\dot{n}	molar flow [mol s^{-1}]
n_{e}	number of transferred electrons for each molecule of fuel [-]
n_{e}^{BV}	number of transferred electrons in Butler-Volmer equation [-]
p	pressure [bar]
P	electric power [W or kW]
PR	pressure ratio [-]
Q_{DH}	district heating production [kJ s^{-1}]
r	ohmic resistance [$\text{k}\Omega \text{ cm}^2$]
R	universal gas constant [$\text{J K}^{-1} \text{ mol}^{-1}$]
T	temperature [K]

U_F	fuel utilization factor for fuel cell [%]
V	potential/overpotential [V]
w	total number of chemical compounds entering the system [-]
\dot{W}	mechanical work [kW]
x	mass fraction [-]
y	molar fraction [-]

Greek Symbols

α	charge transfer coefficient [-]
γ	pre-factor of exchange current density [mA cm ⁻²]
δ	thickness [cm]
Δ	change/difference
ε	heat exchanger effectiveness [%]
η_{CHP}	energy based combined heat and power efficiency [%]
$\eta_{\text{cold gas}}$	gasifier cold gas efficiency [%]
η_{conv}	SOFC conversion efficiency (neglecting fuel utilization) [%]
η_{el}	energy based electrical efficiency [%]
η_{rev}	reversible fuel cell efficiency [%]
η_{SOFC}	overall SOFC efficiency [%]
η_v	voltage efficiency of fuel cell [%]
η_ψ	exergy efficiency [%]
$\eta_{\psi,\text{CHP}}$	exergy based combined heat and power efficiency [%]
$\eta_{\psi,\text{el}}$	exergy based electrical efficiency [%]
$\eta_{\psi,\text{gasifier}}$	exergy based gasifier efficiency [%]
λ	Lagrange multiplier [-]
σ_e	oxygen ion conductivity [S cm ⁻¹]
$\sigma_{e,0}$	pre-factor of ion conductivity [S cm ⁻¹]
$\dot{\Psi}$	exergy flow rate [kW]

Superscripts

0	standard conditions
BV	Butler-Volmer

Subscripts

a	anode
act	activation
c	cathode
C	carbon
cell	single fuel cell
con	consumption
conc	concentration
DH	district heating
e	electrolyte or electrical

elec	electrode
FO	full oxidation
i	interconnect
in	inlet stream
net	netto
ohm	ohmic
out	outlet stream
p	product
PG	product gas
pinch	pinch point
r	reactant
th	thermal
tot	total

Abbreviations

AC	Alternating current
AFC	Alkaline fuel cell
BIGCC	Biomass-based integrated gasification combined cycle
BoP	Balance of plant
CGO	Cerium gadolinium oxide
CHP	Combined heat and power
COS	Carbonyl sulphide
COT	Compressor outlet temperature
DC	Direct current
DH	District heating
DMFC	Direct methanol fuel cell
DNA	Dynamic Network Analysis
DOE	U.S. Department of Energy
DTU	The Technical University of Denmark
GDC	Gadolinium-doped ceria
HHV	Higher heating value
LHV	Lower heating value
LSM	Lanthanum strontium manganite
MCFC	Molten carbonate fuel cell
MGT	Micro gas turbine
NETL	National Energy Technology Laboratory
NREL	National Renewable Energy Laboratory
ORC	Organic Rankine cycle
PAFC	Phosphoric acid fuel cell
PEMFC	Proton exchange membrane fuel cell
ppmv	Parts per million (volume-based)
PR	Pressure ratio
SH	Superheated
SOFC	Solid oxide fuel cell

Nomenclature

S/C	Steam-to-carbon ratio
TIT	Turbine inlet temperature
TOFC	Topsoe Fuel Cell A/S
TOT	Turbine outlet temperature
WGS	Water-gas-shift
YSZ	Yttria-stabilized zirconia

Chapter 1 INTRODUCTION

1.1 MOTIVATION

Development of sustainable and efficient combined heat and power (CHP) plants have gained more attention as climate change, security of the supply, and depletion of fossil fuels have become increasingly well-known issues. Biomass represents a sustainable alternative to fossil fuels because conversion of biomass is carbon-neutral as long as re-planting takes place. Biomass releases the same amount of CO₂ during combustion as previously captured during growth.

Distributed production of biomass feedstocks results in increased cost for fuel transportation, thus local conversion of biomass to electricity and heat can minimize this cost. Still, the most cost-effective biomass use for power generation at present is co-firing in large modern coal power plants [1]. This is due to the high electrical efficiency in modern central power stations compared to decentralized and smaller plants. Modern central coal power plants can obtain net electrical efficiencies of around 50%, while the performances of decentralized and smaller power plants (<30 MW_e) typically suffer from significantly lower electrical efficiencies. Especially decentralized and dedicated biomass CHP plants suffer from low electrical efficiencies, reaching only 30-34% on dry biomass in the typical size of 5-25MW_e [1]. Thus, the main barriers for widespread use of biomass in CHP productions are low conversion efficiency and distributed biomass feedstocks. Therefore, focus should be kept on developing more efficient decentralized CHP plants for use of local biomass feedstocks. Furthermore, decentralized power generation is located closer to the end-user, thus reducing grid losses and expanding the potential for district heating.

Efficient power producing technologies for small-scale production typically include gas engines, gas turbines, and fuel cells – all of which require gase-

ous fuel. An efficient way of reforming biomass into a usable gaseous fuel is by thermochemical processing in a gasifier. Therefore, combining thermal biomass gasification and efficient product gas conversion may enable the design of a sustainable and efficient small-scale CHP plant. The Biomass Gasification Group at The Technical University of Denmark (DTU) has developed a novel and efficient two-stage gasification process (Viking [2]), which produces a very clean product gas from wood chips. The cleanliness of the product gas is very important for many downstream conversion processes, e.g., fuel cells.

Fuel cells present an opportunity to achieve significant efficiency improvements of electricity producing plants. Especially the fuel cell type SOFC (Solid Oxide Fuel Cell) has the advantage of efficient power production. Furthermore, SOFCs operate with high exhaust gas temperature, which can be utilized for additional power generation in heat engines or used for other heating purposes, whether internal in or external to the system. The Danish SOFC developer Topsoe Fuel Cell A/S claims that the electrical efficiency of distributed power generation can be increased from average 40% in traditional power plants to 55% when using SOFC technology [3]. SOFCs can electrochemically convert H_2 and CO to electricity and heat as well as internally reform CH_4 into more H_2 and CO due to their high operating temperature and the presence of a nickel catalyst. Compared to other fuel cell types, these conversion pathways make SOFCs very fuel flexible and ideal for conversion of product gas from thermal gasification.

The usability of a fuel cell is limited without auxiliary components to supply reactants, perform heat management, and do power conditioning. To exploit the great potential of fuel cells, the system of auxiliary components surrounding the fuel cell (BoP – Balance of Plant) needs to be properly designed and optimized. Traditionally, the area of fuel cell research mainly focus on materials, electrochemistry, and stack development, but research within the function and design of the complete system is just as important and will in time gain more focus as the commercial usage of fuel cells approaches.

The combination of thermal gasification and SOFCs is very interesting in the context of utilizing local biomass for decentralized CHP production, as long as the SOFCs can tolerate the alternative gas composition fed to the fuel cells. EU projects (e.g., BioCellus [4] and Green-Fuel-Cell [5]) have investigated the impact on SOFCs when using product gas from thermal biomass gasification. In the BioCellus project, single SOFCs fuelled with product gas from the DTU two-stage gasifier (Viking) were tested, and initial tests showed no significant degradation from impurities even at low steam-to-carbon (S/C) ratios.

A research project dealing with plant layout and optimization of the combination of gasification and SOFC technology can investigate different possibilities of process integration aiming at high net electrical efficiency.

1.2 OBJECTIVES

The overall aim of this research is to contribute to enhanced electrical efficiencies and sustainability in future decentralized CHP plants. For reasons described in the motivation above, the work is focused on studying the potential of combining thermal biomass gasification and SOFCs.

More specifically, the research aims to:

- I. Investigate potential performances of small-scale CHP plant designs based on the two-stage gasification concept (Viking) and downstream power and heat generation from SOFCs.
- II. Develop an SOFC component model with the sufficient level of details to perform plant simulations at various operating conditions.
- III. Locate any optimum of crucial operating parameters with regard to the system performances, and determine the systems' sensitivity to these operating conditions, especially operating conditions related to the SOFCs.
- IV. Identify the best-performing plant concept and complete an optimization of the system layout and operating parameters to reveal the potential performance of two-stage gasification and SOFC hybrid systems.

1.3 METHODOLOGY

The applied methodology for the present research study can be divided into seven steps as listed below. In practice, several steps were conducted in parallel rather than sequentially.

1. Development of three conceptual plant designs based on literature review.
2. Development of a zero-dimensional SOFC model able to handle product gas from thermal biomass gasification as fuel and prepared for integration in a network of component models to enable plant simula-

tions. Calibration of the predicted SOFC performance and completion and assessment of a model test by a parametric study.

3. Development and calibration of a steady-state system-level model of the two-stage gasification plant.
4. Development of complete steady-state system-level models of the three conceptual plant designs.
5. Parametric study of the plant performances by plant simulations.
6. Conduction and assessment of 1st and 2nd law analyses to identify inefficiencies within the best-performing plant of the three studied plant concepts and suggest suitable system optimization efforts.
7. Simulations and assessment of an optimized version of the best-performing plant of the three studied plant concepts.

As mentioned, the aim is to address an enhanced performance of decentralized CHP plants, but the scale of the modelled plant configurations in this study is limited to the largest demonstrated size of the two-stage gasification concept, $\sim 0.5 \text{ MW}_{\text{th}}$ (LHV). The optimized plant design from this work can then directly be used for a future demonstration plant or form the basis for the design of full-scale decentralized CHP plants in the MW_e class based on thermal biomass gasification and SOFCs.

1.4 THESIS OUTLINE

The thesis is divided into eight chapters. Following this first chapter and based on literature review, Chapter 2 includes a description of thermal biomass gasification (including the two-stage gasification concept), SOFCs, and relevant issues concerning coupling of thermal biomass gasification and SOFCs. Furthermore, Chapter 2 describes the history and current development status of gasifier and SOFC hybrid systems. In Chapter 3, three plant concepts are chosen for further investigation and the system layouts are described. Chapter 4 provides a detailed description of the developed SOFC component model, including an electrochemical model predicting the SOFC performance depending on operating conditions. Additionally, a calibration and parametric study of the SOFC model is described in Chapter 4. The developed system-level models of the three plant scenarios are presented in Chapter 5 including modelling and calibration of the two-stage gasification process. In Chapter 6, the simulation results of a parametric system study

are presented and an assessment of the key plant performance data is performed. Chapter 7 includes an optimization of the best-performing plant of the three studied based on 1st and 2nd law analyses. Furthermore, the performances of the original and optimized plants are compared. Finally, Chapter 8 summarizes the findings of this research and gives recommendations for further work.

Chapter 2 BASIS FOR THE STUDY OF COU- PLING GASIFICATION AND SOFCs

To be able to understand the issues of combining thermal gasification of biomass with SOFCs, it is necessary to understand the processes inside a biomass gasifier as well as inside an SOFC. The fundamentals of these technologies are briefly described in this Chapter along with an overview of gas cleaning technologies and a description of the history and state-of-the-art of integrated biomass gasification and SOFC systems.

2.1 THERMAL BIOMASS GASIFICATION

Main processes to convert biomass into power or fuels are biochemical conversion and thermochemical conversion. Biochemical conversion uses the path of fermentation or anaerobic digestion, while thermochemical conversion paths consist of pyrolysis, gasification, and combustion [6]. Combustion produces heat whereas pyrolysis and gasification produce combustible gaseous compounds for easier use in subsequent fuel and/or power production. In the following, the processes inside a gasifier will be described briefly followed by a short overview of gasifier designs and a description of the two-stage gasification concept.

2.1.1 THE PROCESSES INSIDE A GASIFIER

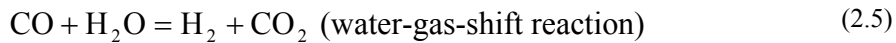
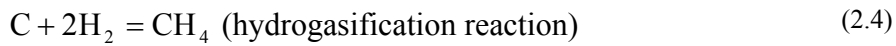
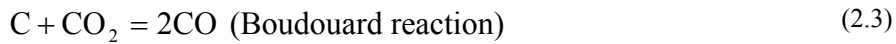
Pyrolysis (devolatilization) decomposes carbonaceous materials by heat in the absence of oxygen. Gases, small quantities of vaporized liquid (tars¹), and a solid residue (char), containing fixed carbon and ash, are produced as

¹ Defined by Milne [7] as: "The organics, produced under thermal or partial-oxidation regimes (gasification) of any organic material, are called "tars" and are generally assumed to be largely aromatic."

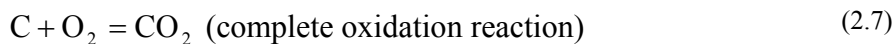
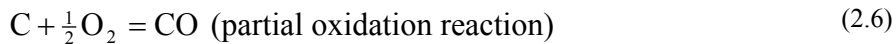
seen in eq. (2.1). The temperature region in which the pyrolysis process takes place is 230-700°C, and the produced gases are H₂, CO, CO₂, CH₄, and H₂O [8].



Gasification further decomposes the fixed carbon into gas compounds in the presence of a gasifying agent and at a higher temperature than the pyrolysis process (typically 800-1100°C) [8]. The gasifying agent can be air, oxygen, steam, and/or carbon dioxide. The main gasification reactions are as follows: [8] [9]



The heat for the endothermic pyrolysis and gasification reactions can be supplied by combustion of char according to eqs. (2.6) and (2.7), and the combustion products can also act as reactants in the gasification reactions:



In a gasifier both pyrolysis, combustion, and gasification occur, and the composition of the produced gas depend on parameters such as gasifier design, fuel composition, moisture content in fuel, gasifying agent, operating temperature, and operating pressure of the gasifier [8]. The gasifier can also be heated by external heat sources. External heating is called allothermal gasification, whereas internal heating, by eqs. (2.6) and (2.7), is called auto-thermal gasification.

Generally, thermal gasification of biomass leads to five primary contaminants in the product gas; particulates, tars, sulphur, alkali compounds, and nitrogen-containing compounds. Particulates are solid-phase materials entrained in the produced gas flow and typically consist of ash or unconverted carbon. Tars cover a range of complex higher hydrocarbons or oxidized organics formed in the pyrolysis process, and they typically leave the gasifier

as vaporized liquids. At lower temperatures many tar compounds condense, entailing risk of plugging or fouling equipment. Sulphur compounds in the produced gas originate from the sulphur content in gasifier feedstock. Biomass feedstocks have low sulphur content compared to coal. Minerals in the ash of the feedstock vaporize at temperatures about 700°C, and alkali compounds can be formed. These alkali compounds condensate into/on solids in the gas flow at around 650°C and can deposit and/or be corrosive to metal surfaces. Proper removal of particulates at lower temperatures will significantly reduce alkali loading. Ammonia is the primary nitrogen-containing compound formed, and it originates from the nitrogen content in the feedstock. Usually, ammonia in the product gas is undesired because it leads to NO_x formation when burned. [10]

Both particulate and tar loading are very depended on the gasifier design, whereas sulphur, alkali, and nitrogen-containing compounds depend on the feedstock. The heating value of tars is not negligible, so it is desired that they are converted in the gasifier or utilized in some way. More details on contaminants from biomass gasification can be found in the DOE/NREL report by Stevens [10], and comments on gas cleaning techniques are given later in this Chapter.

2.1.2 GASIFIER DESIGNS

Generally gasifiers can be divided into two design types; fixed bed and moving bed. Fixed bed gasifiers are characterized by a reactor design where a solid fuel feed is added in the top and stationary placed in a bed as shown in Figure 2.1. Fixed bed gasifiers can be updraft or downdraft gasifiers, and the difference is the direction of the gasifying agent flow compared to the solid fuel (co-current vs. counter-current), also shown in Figure 2.1. In the updraft gasifier, the partial oxidation takes place in the bottom heating the gasification of char, the pyrolysis process, and the drying zone on top. The produced gas is cooled through the drying zone, and tars and different hydrocarbons from the pyrolysis process escape easier because they do not pass through the hot char bed or the oxidation zone. In the downdraft gasifier, the partial oxidation takes place between the pyrolysis and char gasification zones. Here, the pyrolysis products pass through the oxidation zone and the hot char bed reducing the tars and hydrocarbons. Therefore, the temperature of the product gas leaving the downdraft gasifier is higher than that of the updraft design. [10]

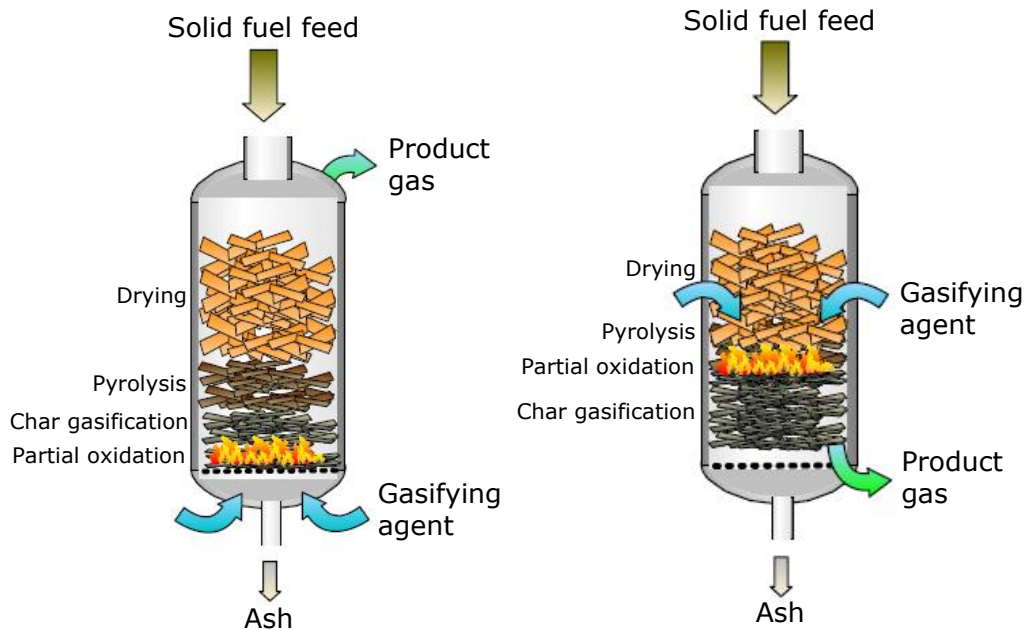


Figure 2.1: Sketches of an updraft (left) and a downdraft (right) autothermal fixed bed gasifier [figures of unknown origin].

The lower temperature of the exiting product gas in the updraft gasifier ensures a more efficient gasification than in the downdraft gasifier because the heat losses are lower. On the other hand, the downdraft gasifier produces a cleaner gas than the updraft gasifier (see Table 2.1). Fixed bed gasifiers can be built in small to medium scale (up to a few MW_{th}) [10].

Table 2.1: Particulate and tar levels from different biomass gasifier designs [10].

Gasifier type	Particulate loading [g Nm ⁻³]	Tar loading [g Nm ⁻³]
Fixed bed		
Downdraft	0.1-0.2	0.1-1.2
Updraft	0.1-1.0	20-100
Moving bed		
Bubbling fluidized bed	2-20	1-15
Circulating fluidized bed	10-35	1-15

Moving bed gasifiers are defined as gasifiers where the bed material is either fluidized by the gasifying agent or entrained in a gas flow and co-fed with an oxidant to a reactor working as a burner operating at fuel rich conditions. Fluidized bed gasifiers can be bubbling fluidized bed gasifiers or circulating fluidized bed gasifiers. In the bubbling fluidized bed gasifier, the bed material is agitated by the gasifying agent flowing through it. In the circulating fluidized bed gasifier, the bed material is circulated between the

gasifier and typically a cyclone separating gas from bed material. The bed material is recirculated to the gasifier, and heating of the gasifier can either be by partial oxidation in the gasifier or by indirect heating through heating of the circulating bed material. Turbulence in the moving bed gasifiers ensures effective mixing and heat transfer, but also higher levels of particulates in the product gas (see Table 2.1). The tar loading is higher than the downdraft fixed bed gasifier but lower than the updraft gasifier, and the product gas leaves the moving bed gasifiers at relatively high temperatures. Moving bed gasifiers can be sized for medium-scale to large-scale facilities (MW_{th} scale). [10]

2.1.3 TWO-STAGE GASIFICATION

In the so-called Viking gasifier ($75 \text{ kW}_{\text{th}}$ [2]) demonstrated by the Biomass Gasification Group at the Technical University of Denmark, the pyrolysis and gasification processes are divided into two separate reactors as depicted in Figure 2.2. Wet biomass (wood chips) is fuelled to the first reactor where drying and pyrolysis takes place, before the pyrolysis products (600°C) are fed to the second reactor, which is a downdraft fixed bed char gasifier. The drying and pyrolysis reactor is externally heated, in this case by the exhaust gas from a gas engine fuelled with the producer gas. In between pyrolysis and char gasification, partial oxidation of the pyrolysis products provides the heat for the endothermic char gasification reactions by addition of pre-heated air, and a temperature of $1100\text{--}1300^\circ\text{C}$ is reached in this zone. Char is gasified in the fixed bed, where H_2O and CO_2 act as gasifying agents in the char gasification reactions at temperatures of $1100\text{--}800^\circ\text{C}$ [11]. The Viking gasifier operates near atmospheric pressure.

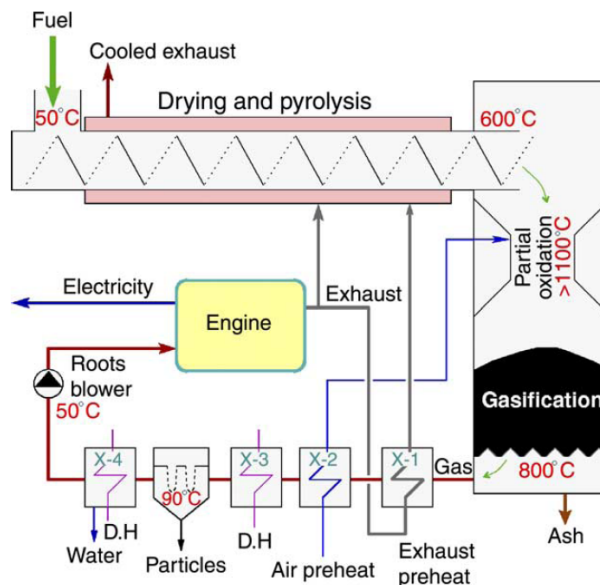


Figure 2.2: Flow sheet of the Viking gasifier [2].

Tars formed in the pyrolysis process are cracked in the high-temperature partial oxidation zone reducing the tar content by a factor of 100, and as the partially oxidized pyrolysis products pass through the char bed, the tar loading is further reduced by a factor of 100 [2]. Thus, the tar content in the product gas leaving the gasifier is extremely low. In one paper [2] from the developers of the Viking gasifier it was stated that the tar content in the produced gas was below 15 mg Nm^{-3} , and in another paper [11], the Viking developers presented results from three different tar measurement techniques, where only one of the three techniques could detect $0.02\text{-}0.1 \text{ mg Nm}^{-3}$ naphthalene in the raw gas before gas cleaning. The key to this low tar content is the high-temperature cracking in the partial oxidation zone and the reduction when passing through the char bed. Introducing the correct amount of air, ensuring good mixing with the pyrolysis gas in the partial oxidation zone, and avoiding any of the partially oxidized pyrolysis gas to bypass the char bed are crucial issues for the level of success in producing a low tar gas [12].

The raw product gas leaves the char gasification reactor at 800°C and is cooled in two preheating steps and a district heating production, before it is cleaned from particulates in a bag filter at approximately 90°C (slightly above the water dew point) [2]. Hereafter, the cleaned gas is further cooled and water is condensed. More district heating is produced in this step. The flow of product gas is ensured by a blower, and the resulting dry gas composition and lower heating value of the clean product gas are as stated in Table 2.2. Also the cold gas efficiency of the gasifier and the net electrical efficiency of the system including the gas engine are shown in Table 2.2, and their definitions can be found in eqs. (2.8) and (2.9). As previously mentioned, the downdraft gasifier design usually obtains lower cold gas efficiency than the updraft design because of the higher outlet temperature and thereby heat losses. Since the drying and pyrolysis processes are externally heated by waste heat, the resulting cold gas efficiency is high compared to traditional downdraft gasifiers.

Table 2.2: Dry gas composition, LHV as well as efficiencies for the Viking gasifier [11].

H ₂ (vol-%)	30.5
CO (vol-%)	19.6
CO ₂ (vol-%)	15.4
CH ₄ (vol-%)	1.16
N ₂ (vol-%)	33.3
LHV (MJ kg ⁻¹)	6.2
Cold gas efficiency	93%
Net electrical efficiency	25%

$$\eta_{\text{cold gas}} = \frac{\dot{m}_{\text{cold product gas}} LHV_{\text{cold product gas}}}{\dot{m}_{\text{biomass}} LHV_{\text{biomass}}} \quad (2.8)$$

$$\eta_{\text{el}} = \frac{P_{\text{net}}}{\dot{m}_{\text{biomass}} LHV_{\text{biomass}}} \quad (2.9)$$

Some contaminants are present in the cleaned gas and measurements on these are listed in Table 2.3. As expected, the level of impurities from a downdraft fixed bed gasifier is low (cf., Table 2.1). However, the very low tar content is ensured by the tar destruction technique used in the two-stage gasification approach. The amount of sulphur in the product gas is directly depended on the sulphur content in the biomass feedstock. By means of the two-stage gasification process, extensive gas cleaning can be avoided. Thus, the plant complexity can potentially be kept low (and thereby also reduce the plant cost).

Table 2.3: Measured contaminants in producer gas after bag filter and condenser.

Tars (mg Nm ⁻³)	<1
Naphtalene [11]+[13]	0.02-0.25
Anthracene [13]	0.05-0.08
Sulphur (ppmv)	<2
H ₂ S [13]	<1
COS [13]	0.930
Ammonia (mg Nm ⁻³) [11]	60-140 ^a
Dust (mg Nm ⁻³) [14]	<5

^a 520-540 mg Nm⁻³ in the raw gas.

The Viking gasifier is a demonstration plant with a thermal biomass input of only 75 kW_{th}, but the concept is scalable up to the range of 3-10 MW_{th} [15]. A sketch of the medium size two-stage gasification concept is depicted in Figure 2.3. Here, the biomass drying and pyrolysis are divided into separate reactors, where the drying is done by superheated steam produced from the gas engine exhaust, and the pyrolysis reactor is heated by the hot product gas. The reactor size of the dryer and the residence time in the dryer are substantially reduced, when the drying medium is in direct contact with the biomass [16].

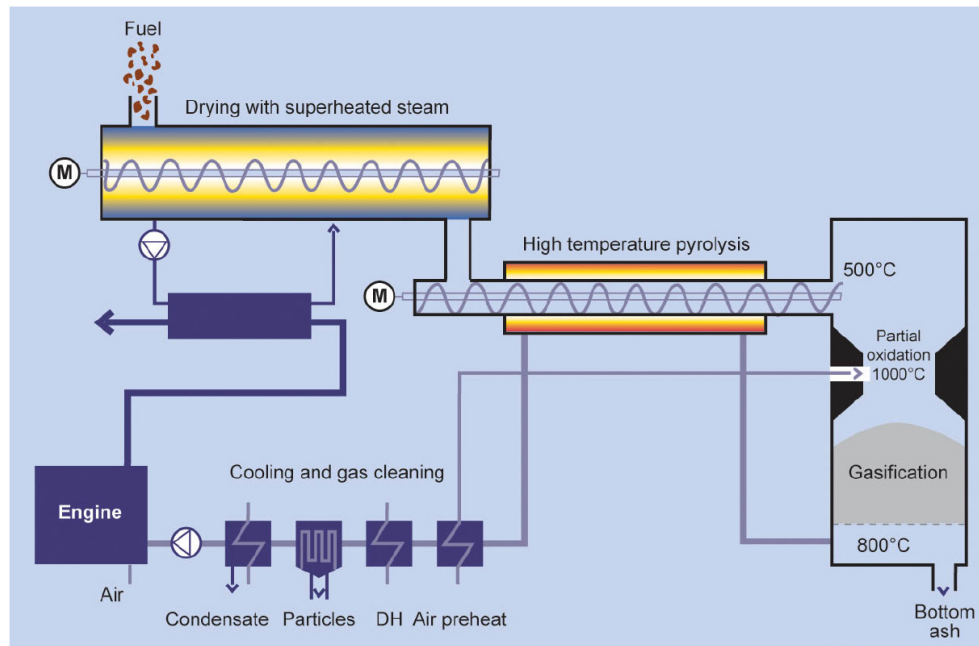


Figure 2.3: The two-stage gasification concept upscaled to 3-10 MW_{th} [15].

A 600 kW_{th}/200 kW_e pilot plant of the two-stage gasification concept has been built in 2007 by DTU, COWI, and Weiss [16], proving the scalability of this gasification concept.

2.2 SOLID OXIDE FUEL CELLS

A fuel cell is an energy converting technology producing electricity directly from oxidizing a fuel through electrochemical reactions. Various types of fuel cells exist with different advantages and disadvantages, but generally they are known for their high efficiency, simplicity, low emissions, and silent operation [17]. Besides that, fuel cells are also efficient when operating at part load.

A typical way to characterize a fuel cell type is by its electrolyte material. An overview of the most common fuel cell types and their characteristics is presented in Table 2.4.

The high-temperature fuel cells (MCFC and SOFC) have the greatest potential to be integrated in larger CHP systems, as shown in Figure 2.4, because the high-quality heat from the fuel cells can be utilized for additional power production in a bottoming cycle or for other heating purposes. Therefore only these high-temperature fuel cell types are relevant to this study.

Table 2.4: Fuel cell types and their characteristics.

Fuel cell type	Mobile ion [17]	Operating temperature [17]	Direct fuels ^a
Alkaline (AFC)	OH^-	50-200°C	H_2
Proton exchange membrane (PEMFC)	H^+	30-100°C	H_2
Direct methanol (DMFC)	H^+	20-90°C	CH_3OH
Phosphoric acid (PAFC)	H^+	~220°C	H_2
Molten carbonate (MCFC)	CO_3^{2-}	~650°C	H_2, CO
Solid oxide (SOFC)	O^{2-}	650 ^b -1000°C	H_2, CO

^a Here defined as the fuels that can be electrochemically converted in the fuel cell.

^b Research efforts are trying to lower the operating temperature of SOFCs to reduce material costs.

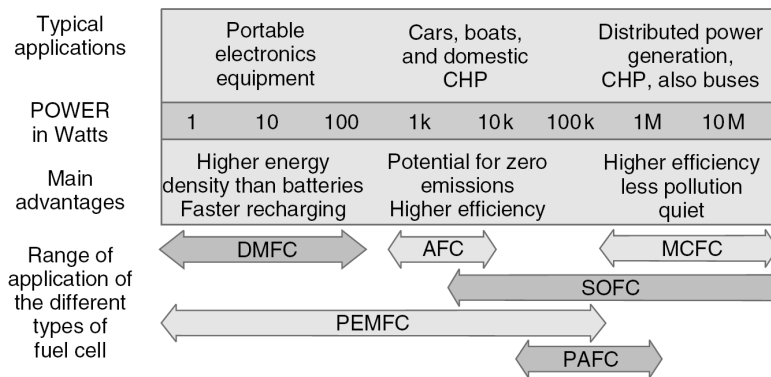


Figure 2.4: Scale of applications for different fuel cell types [17].

This study is confined to looking at the SOFC type only and not the MCFC, even though MCFCs also have the potential to be a part of future CHP plants.

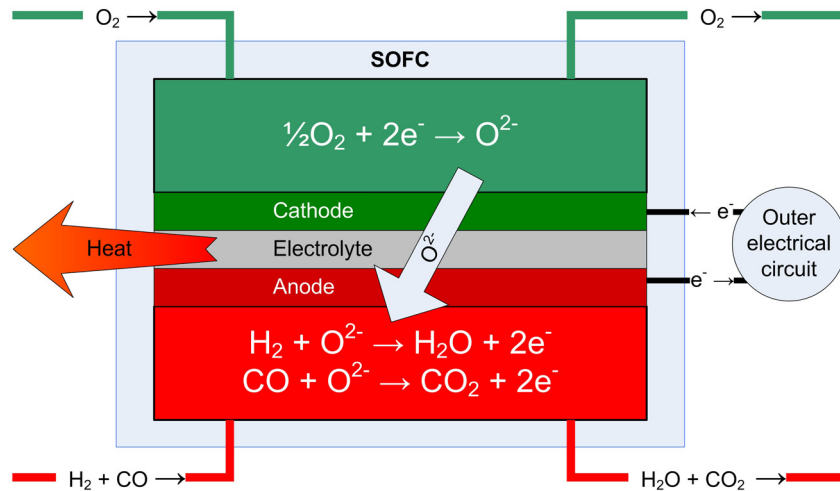
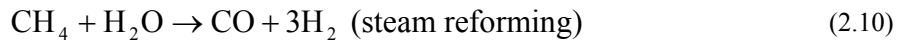


Figure 2.5: A sketch of a solid oxide fuel cell and the electrode reactions.

As seen in Figure 2.5, the SOFC can both electrochemically convert H_2 and CO on the nickel containing anode by reaction with oxygen ions coming from the cathode side through the ion conducting electrolyte. Oxygen ions are the mobile ions in SOFCs, whereas other fuel cell types have other mobile ions (see Table 2.4). Besides H_2O and CO_2 , the anode reactions produce electrons, which are led through an outer electrical circuit to meet with oxygen on the cathode and produce oxygen ions. The transport of electrons is characterized as an electrical current.

Furthermore, SOFCs can internally reform CH_4 and NH_3 into H_2 and CO due to their high operating temperature and the presence of a nickel catalyst. This makes SOFCs very fuel flexible and ideal for converting gas from gasifiers, or other reforming processes, compared to other fuel cell types. The reforming reactions are shown in eq. (2.10) [18] and eq. (2.11) [19]. Additionally, the water-gas-shift reaction, as shown in eq. (2.5), will balance the ratio between H_2 and CO depending on the operating conditions.



A single fuel cell generates a potential of the level of 1 V, so to reach a higher potential they are connected in series in stacks. Several cell designs exist, but the most common two are the planar and tubular design. More general information on fuel cells and stack designs can be found in Larminie and Dicks [17] and more specific on SOFCs in Singhal and Kendall [18].

In Denmark, the players within SOFC R&D and production are Risø DTU (National Laboratory for Sustainable Energy) and Topsoe Fuel Cell A/S (TOFC). The SOFC type developed at Risø and TOFC is of the planar design. It is anode-supported and the anode consists of nickel and yttria-stabilized zirconia (YSZ), the electrolyte of YSZ and the cathode of lanthanum strontium manganite (LSM) and YSZ [20].

2.2.1 TOLERANCE TO IMPURITIES

SOFCs have certain tolerances to different contaminants in the fuel fed to the anode. Among these are sulphur compounds, which are poisonous to the nickel anode when present. At the anode conditions, all sulphur compounds will be converted into hydrogen sulphide (H_2S), which is chemisorbed on the nickel surface [21], thus passivating the active sites. Rostrup-Nielsen et al. [21] indicated that the electrochemical reactions are less sensitive to sulphur poisoning than the internal reforming reactions, which are highly affected. They also reported that at 800°C , addition of 10 ppmv of H_2S in the fuel feed (reformer gas) to a 10-cell TOFC stack had no impact on the SOFC performance, while 50 ppmv of H_2S resulted in a reduced cell potential. Rasmussen and Hagen [22] demonstrated an initial cell voltage drop of 10% from adding 2 ppmv H_2S at 850°C using hydrogen as fuel at 1000 mA cm^{-2} . The poisoning effect increase with decreasing temperature and also factors such as fuel, current density, time, and sulphur concentration affects the impact [22] [23], so it seems to be difficult to find consensus on a specific tolerance level to H_2S for nickel based SOFC anodes. At least the poisonous impact from H_2S is reversible at moderate levels (<40 ppmv), meaning that the SOFC performance will recover when the sulphur contaminant is removed [21] [22]. Development of sulphur tolerant anodes is a research field of increasing interest [24], and some have shown promising results [25] [26]. This development could further improve the fuel flexibility of SOFCs and remove the need for a sulphur clean-up step before feeding the fuel to the anode. Generally, the impact of sulphur poisoning seems to be a potential reduction, so to certain extend, the problem could be dealt with by cell or stack dimensioning.

Chlorine compounds such as the hydrogen halide HCl (hydrogen chloride) and alkali halides are usually represented by HCl only [26]. HCl is poisonous to nickel anodes and is expected to affect the anode by similar mechanisms as H_2S , but the extent of degradation from HCl is less [27]. The degradation is also reversible as H_2S . Based on literature and own research, Tremblay et al. [27] state that HCl will not reduce the SOFC performance when below a concentration of 1 ppm. Stable performance could be achieved with 20 ppm HCl in the fuel [27], so to certain extend HCl poisoning could also be dealt with by dimensioning as for H_2S poisoning. Aravind

et al. [26] showed promising test results with a Ni/GDC anode tolerating up to 9 ppm of H_2S and HCl .

Tolerance to particulates is not well-described in the open literature. Particulates of ash and/or unconverted carbon can deposit on the anode, thus blocking the gas diffusion paths, blocking catalytic sites, or provoke anode layer delamination due to mechanically induced tensions [28]. Hofmann et al. [28] made tests on SOFCs (Ni/GDC anode) with real product gas from biomass gasification and accidentally exposed the Ni/GDC anode to ash and char particulates smaller than 5-10 μm in diameter during operation. Normally particulates were removed by first a cyclone and then a metal candle filter, but the metal candle filter failed in one of the tests. Particulates were later identified on the surface of the anode. No contaminants were observed on the anode when the metal candle filter was functioning.

Tars are not necessarily poisonous to SOFCs. Presence of tars can induce carbon deposition on nickel containing anodes at certain conditions, which results in degradation of the SOFC performance. This has been reported by Singh et al. [29] in a theoretical study. Solid carbon is formed through the Boudouard reaction and methane cracking (going from right to left in eqs. (2.3) and (2.4)). The extend of carbon deposition depends on various parameters such as temperature, S/C ratio, current density, and anode material. The carbon deposition decreases with the increase of S/C ratio or with the increase of current density [29]. Mermelstein et al. [30] showed by experiments, that carbon deposition was reduced significantly in both Ni/YSZ and Ni/CGO anodes fed with 15 mg Nm^{-3} tars in a H_2/N_2 fuel mix at 765°C , when the S/C ratio was greater than 1. Higher fuel utilization ($>50\%$) should make SOFCs able to operate at lower S/C ratios with reduced carbon formation because H_2O and CO_2 produced from the electrochemical reactions will suppress carbon deposition and/or remove deposited carbon [30]. Hofmann et al. [14] used C-H-O ternary diagrams to predict and experiments to show, that solid carbon formation was not formed when fuelling an SOFC with product gas from the Viking gasifier at a temperature of 850°C , a current density of 260 mA cm^{-2} , a fuel utilization of 30%, and a S/C ratio of 0.5. This was also due to the very low tar content in the product gas from the Viking gasifier and an activated carbon filter removing some of the tars. 0.17 mg Nm^{-3} of naphthalene was present in the gas at the anode inlet. According to the statement by [30] above, it should be possible to operate at an even lower S/C ratio than 0.5 without carbon deposition, if the fuel utilization of 30% was increased significantly.

2.3 OVERVIEW OF GAS CLEANING

Cleaning of the produced gas is often essential for downstream end-use technologies. To be able to meet the requirements of these technologies different clean-up steps should be considered.

To remove particulates, cyclones, barrier filters, electrostatic filter, or wet scrubbers can be used. Cyclones can remove up to 90% of particulates larger than 5 μm in diameter at high temperatures (only limited by material constraints). Barrier filters can remove particulates of 0.5 to 100 μm in size. Barrier filters can be constructed of metals or ceramics for hot gas cleaning, or woven materials (bag filters) for cleaning up to 350°C. Electrostatic filters can operate up to 500°C or more and can remove 99% of particulates smaller than 0.1 μm , while wet scrubbers are very efficient for particulates larger than 1 μm , but at temperatures below 100°C. [10]

Tar loading is very much depended on gasifier design, so first of all, tars should be limited by design considerations. Otherwise, tars can be dealt with by physical, catalytic, and thermal removal. Through the physical tar removal route, the tars are condensed and filtered. Catalytic destruction decomposes tars to additional product gas either in situ or in a downstream reactor. The non-metallic catalyst dolomite has proven to remove 95-99% of tars at 750-900°C under laboratory conditions. Thermal destruction decomposes tars to additional product gas at temperatures above 1200°C and without a catalyst. [10]

Thermal destruction is the technique used in the two-stage Viking gasifier between the pyrolysis process and char gasification.

Concerning sulphur, the relatively small amounts of H_2S from biomass gasification can be removed by absorption onto metal oxide pellets in a bed at about 480°C [10]. Dayton et al. [31] report that the upper temperature limit for the most common H_2S sorbent ZnO is 600°C. COS is on the other hand more effectively adsorbed in an active carbon bed. Sakanishi et al. [32] suggest a metal-supported active carbon bed for simultaneous removal of H_2S and COS .

Commercial H_2S absorption by ZnO is presently available. Removal is recommended at 300-400°C, but can also be done from ambient conditions up to 450°C. Even combined removal of H_2S and COS is available. [33]

Alkali compounds condense into solids or on particulates below 650°C. Hereby alkali compounds can be removed in the same manner as particulates. Particulate size can be below 5 μm , so cyclones will not be effective. Research is being conducted on alkali traps for removing alkali compounds at high temperature. [10]

From the SOFC point of view, it is not needed to remove ammonia, since it can be converted in the fuel cell as described earlier. Therefore, gas conditioning techniques for ammonia removal are not investigated here.

Hot gas cleaning technologies have gained increasing interest because cooling of the hot producer gas from the gasifier can be avoided. This can be beneficial when coupling gasification with other high-temperature technologies because of better heat management.

2.4 HISTORY AND DEVELOPMENT STATUS

Gasification and fuel cells were first combined with the intention to improve coal to electricity efficiencies. In the early 1980s, advanced coal gasification and MCFC (Molten Carbonate Fuel Cell) systems were explored under DOE [34], but in 1988 Reed and Das [35] mentioned in their book on biomass gasifier systems that fuel cells are a potentially interesting technology to generate electricity from biomass derived producer gas.

The first to report on a thermodynamic analysis of the combination of a biomass gasifier and SOFCs were Alderucci et al. in 1994 [36]. In this early publication a fluidized bed gasifier, using either steam or CO₂ as gasifying agent, was studied, and equilibrium calculations were used to predict the conversion levels in the gasifier. The SOFC electrical efficiency was calculated at different gasifier operating conditions such as the gasifier operating temperature. In the case of a gasifier operating temperature of 700°C, the SOFC performed with electrical efficiencies of 47% using steam as gasifying agent and 51% using CO₂. Efficiencies of the entire system were not calculated.

The coupling of biomass gasification and high temperature fuel cells was also mentioned by Craig and Mann [37] in 1996 in a reported study on BIGCC (Biomass-based Integrated Gasification Combined Cycle) as a future potentially high-efficient CHP production from biomass.

A thorough design study of an SOFC and gas turbine system combined with biomass gasification was published in 2000 by Barchewitz and Palsson [38]. This work calculated total system efficiencies of a plant producing 4-5 MW_e. The gasifier was a pressurized autothermal air-blown circulating fluidized bed gasifier and the SOFCs were of planar design. It was assumed that all tars were cracked inside the gasifier, which is most unlikely in this type of gasifier. Barchewitz and Palsson referred to Ståhl and Neergaard [39], while Ståhl and Neergaard reported on problems associated with tars

in the product gas. A recuperator recovering heat from the gas turbine outlet was included and the resulting electrical system efficiency was found to be 58.5% at an optimal pressure of 2.65 bar. The low operating pressure was caused by the recuperative loop (see, e.g., Saravanamuttoo et al. [40] or a brief explanation in the end of Chapter 3). By reducing the SOFC stack size and increasing the gas turbine output, the efficiency was reduced to 55.1% at 5.25 bar, but the capital costs were also reduced.

Hutton et al. [41] reported in 2003 on a feasibility study of a thermally integrated downdraft biomass gasifier and SOFC system, where a net electrical efficiency of 38% (based on HHV) was predicted. The thermal integration featured heating of the gasifier by the burned off gases from the SOFCs, reducing or neglecting the need for air supply to the gasifier (depended on the moisture content in the woody biomass).

In 2004, Omosun et al. [42] modelled two biomass-fuelled SOFC systems where the effect of hot versus cold gas cleaning on system efficiencies and costs were studied. The electrical system efficiencies were similar at around 22%, but the hot gas cleaning showed better heat management and thereby overall cogeneration efficiency. The low electrical efficiency was due to low fuel utilization in the SOFC (set to 50%) and the fact that the SOFC off gases were burned and used for district heating production and drying of biomass. Compared to the work of Barchewitz and Palsson, the efficiencies are substantially lower pointing out the importance of utilizing the SOFC off gases in a proper manner. In the case of Barchewitz and Palsson, this is done in a recuperated gas turbine. Additionally, removal of sulphur compounds was not included in the study by Omosun et al. in opposition to tars, particulates and alkali compounds, even though sulphur is very poisonous to SOFCs.

Sucipta et al. [43] published in 2007 a performance analysis of a tubular SOFC and recuperated MGT hybrid system fuelled with gasified biomass using air, oxygen, or steam as gasifying agent. A scenario using pure methane was used as reference. Electrical efficiencies of the hybrid system without the gasification process were found to be 46.4%, 48.9%, and 50.8% for air, oxygen, and steam, respectively. The reference scenario using pure methane performed 59%. The main reasons for the lower performance in the biomass scenarios were the lower heating value of and inactive species in the biomass producer gas.

In 2008, Fryda et al. [44] modelled an autothermal (air) biomass gasifier integrated with SOFCs and/or a micro gas turbine with a biomass throughput of 200 kg/h (almost 900 kW_{th} (LHV)). The combination of a gasifier, SOFCs, and a micro gas turbine achieved the highest electrical efficiency of

40.6%. Surprisingly, the gasifier and micro gas turbine system outperformed the gasifier and SOFC combination with an electrical efficiency of 26.1% versus 20.0%. An electrical efficiency below 20% of the SOFC in the gasifier and SOFC combination seems unrealistically low if dimensioned and operated properly.

As seen from the above descriptions of studies on biomass gasification and SOFC hybrid systems, this specific field is heavily based on modelling studies. Experimental investigations are usually limited to lab scale tests of single SOFCs operated on biomass derived producer gas, typically to test SOFC tolerance to trace species [14] [26] [28] [45] [46]. Oudhuis et al. [47] reported on proof-of-principle lab-scale tests with an oxygen-blown biomass gasifier and a 5-cell SOFC stack (Sulzer HEXIS) for up to 48 hours of operation. The SOFC stack achieved an electrical efficiency of 41% at a fuel utilization of 80%.

Recently, two EU projects, BioCellus [4] and Green-Fuel-Cell [5], have been completed. Both projects dealt with issues of combining biomass gasification and SOFCs, and special focus was on obtaining a clean producer gas from appropriate gasifier design and/or hot gas cleaning. Thermal integration between an allothermal biomass gasifier and tubular SOFCs by means of liquid metal heat pipes transferring the excess heat from the SOFCs to the gasifier comprise a novel coupling for small-scale CHP, which were also presented in the BioCellus project [48] [49] [50] [51]. Based on a modelling study, Panopoulos et al. [50] report that a total electrical efficiency of 36% (32% by exergy [51]) at 70% fuel utilization and a current density of 250 mA cm^{-2} can be achieved to produce 140 kW_e . Successful testing of single cell SOFCs operated on producer gas from the Viking gasifier for 150 hours were also conducted in the BioCellus framework [14].

2.5 KEY ISSUES RELEVANT TO THIS STUDY

From the literature some important points have shown when it comes to combining thermal biomass gasification and SOFCs in a sustainable and efficient decentralized CHP production.

Providing a clean producer gas which meets the requirements of the SOFC is essential. This can be obtained partly by proper gasifier design and also by downstream gas conditioning. Especially the tar and particulate loadings can be reduced from appropriate gasifier design, whereas compounds origi-

nating from inorganics in the biomass feedstock are less sensitive to gasifier design.

Utilization of SOFC off gases is also important to obtain high system efficiency, since not all producer gas is converted in the SOFC. Therefore, the SOFC off gases contain unconverted fuel and also high-quality heat, which can be exploited for additional power generation or heating purposes. Several studies have shown that gas turbine technology can exploit the SOFC off gases to produce additional power.

Heat management is also of great importance to the resulting system efficiency, whether it is within in the gasification process, the SOFC system, or any additional parts of the system, or it is between the different system parts. In this context, methods for cooling the SOFC should get attention, and if a gas turbine is included in the system, use of a recuperator have shown to be beneficial. Alternatively, the hot gas turbine exhaust can be used to generate steam for a Rankine cycle if the plant size is big enough.

The cold gas efficiency of the gasifier should be as high as possible, since it is hard to compensate for losses from the gasification process in the latter parts of the system. This was also shown in [52].

Furthermore it must be expected, that keeping the system design simple and choosing state-of-the-art components will contribute to the design of an efficient CHP plant with reasonable investment and maintenance costs.

Chapter 3 INVESTIGATED PLANT CONFIGURATIONS

Based on the literature review forming a basis for this study in the previous chapter, three conceptual system layouts have been chosen for further investigation. These are all based on thermal gasification of biomass, as in the Viking two-stage gasification concept, supplying producer gas for downstream electricity generation. The reason for choosing the Viking gasifier concept is the production of a very clean gas from this plant reducing the need for extensive gas conditioning. Furthermore, the cold gas efficiency is very high, forming the basis for an efficient plant. In spite of the use of a downdraft gasifier reactor in the Viking concept, the cold gas efficiency is very high, and this is due to external heating of the reactor where drying and pyrolysis takes place (only where drying takes place in the upscaled concept, cf., Figure 2.3). Hereby, the need for adding air to heat the gasifier is reduced, and less of the feed to the gasifier is burned. The product gas is also less diluted with N_2 .

Downstream the biomass gasification, product gas is converted to electricity and heat for district heating purposes. This is done in three different scenarios; using only a micro gas turbine (MGT), using only SOFCs, or using both combined. Studying these three scenarios is expected to give an overview of the benefit from choosing an efficient SOFC over a conventional technology and also the advantage of combining these to gain even higher electric power yield. The potential performance of combining biomass gasification, by the two-stage concept, and SOFCs should also be revealed.

Since the hybrid system should work as a decentralized CHP plant, the size should be in the range of 5-30MW_e (some decentralized plants can be smaller or larger) [53]. The size chosen in this study, though, is determined by the currently available two-stage gasifier size of around 0.5 MW_{th} (as previously mentioned a 600 kW_{th}/200 kW_e pilot plant has been demon-

strated [16]). Thus, the chosen size in this study aims at very small decentralized CHP plants and future demonstration plants. Nevertheless, it must be expected that larger plants will perform at least as good as the chosen plant size. It is assumed that the cold gas efficiency and product gas composition are the same as for the Viking gasifier (75 kW_{th}). It is expected that the two-stage gasification concept is scalable up to 10 MW_{th} as depicted in Figure 2.3, but also even further up to 50 MW_{th} using a fluid bed design [15], so the potential for designing decentralized CHP plants based on gasification by the two-stage concept is present. The chosen plant size is also sufficient for the ability to include a MGT in the system, but not big enough to include a steam based Rankine cycle downstream the gas turbine. Instead, the excess heat in the gas turbine exhaust is recuperated to the compressed air intake. Since the thermal plant input is fixed, the electric power production is depended on the electrical efficiency of the hybrid system.

Flow sheets of the three conceptual scenarios are sketched in Figure 3.1, and the alternative flow directions in the scenarios using only a MGT or only SOFCs are indicated by two kinds of dashed lines.

Wet wood is fed to the dryer, producing dry wood and steam, which both are led to the gasifier. For reasons of simplification, the pyrolysis takes place inside the gasification reactor in this modelling study. In the demonstrated 75 kW_{th} Viking gasifier, the drying and pyrolysis reactor is heated by the gas engine exhaust gases, but around 80% of the heat supplied to this reactor is used for drying [16]. Furthermore, some of the gas engine exhaust is superheated by the hot product gas from the gasifier before it is sent to the drying and pyrolysis reactor as seen in Figure 2.2. It is therefore assumed that the pyrolysis process is not heated by external heat from the gas engine, but by heat from the gasifier, which is also the case in the upscaled version of the two-stage concept depicted in Figure 2.3. Thus, only the drying process is externally heated in this investigation. Since change of the outlet temperature from the modelled gasification reactor will affect the raw gas composition, the air input to the gasification reactor is preheated more in this study than in the demonstrated Viking gasifier to compensate for the heat consumption from the endothermic pyrolysis process inside the gasifier. The temperature of the slightly cooled product gas after the air preheater should be the same in this study and in the demonstrated two-stage gasification concept, but measurements on this temperature is unknown to the author. From a system point of view, it is just important to obtain the correct cold gas efficiency and gas composition, unless additional thermal integration between the gasification and power generating part of the system is necessary.

As for the Viking gasifier, a bag filter removing particulates is the only gas cleaning device in the considered system. The product gas is cooled to 90°C before it is led through the filter. It is assumed that no alkali compounds leave the gasifier plant entrained in the producer gas flow, since all alkalis should be condensed at such low temperatures, thus removed along with particulates in the bag filter. The sulphur content is expected to be very low (see Table 2.3), so no sulphur clean-up step is included. If it was found necessary, a ZnO bed could be located somewhere after the gasifier air preheater depending on the preferred operating temperature of such a sulphur removal unit. Introducing a ZnO bed would not affect the rest of the system by other means than a small pressure drop and heat loss. If a ZnO bed was used, a S/C ratio above 1.66 at 400°C should be kept to avoid carbon deposition [54], thus, depending on the chosen operation temperature of the ZnO bed, addition of water might be necessary. As a last step in the biomass gasification process, the product gas is cooled to condense some of the water reaching a product gas temperature of around 50°C.

As mentioned, the power generating part of the system has three scenarios; one where all components in Figure 3.1 are in use (which from now on will be referred to as the SOFC-MGT configuration), and two where some components are bypassed. In one of the latter scenarios the SOFCs including preheaters are bypassed, by which all electric power generation is provided by the MGT, and this scenario is named the MGT configuration. The last scenario bypasses the MGT expander and recuperator and only uses the SOFCs for power generation, and this scenario is from now on referred to as the SOFC configuration.

In all three scenarios, the product gas is supplied by a product gas compressor and the air by an air compressor. Suction from the product gas compressor ensures gas flow in the gasification process. In the SOFC configuration, the two compressors are working as blowers, since the power generating system is not pressurized, contrary to the MGT and SOFC-MGT configurations. The SOFC feeds are preheated by the SOFC off gases (800°C) to be able to keep the temperature difference through the SOFCs at an acceptable level, and subsequently the off gases are combusted in a burner to convert remaining combustibles. The hot flue gas from the burner is either utilized for additional power generation in the MGT (MGT and SOFC-MGT configurations) or for district heating production (SOFC configuration).

When the MGT is used, a recuperator is included for additional preheating of the air supplied to the SOFC cathode. If the cathode inlet and outlet temperatures are unchanged, the impact of including a recuperator will be an increased temperature of the cathode off gas introduced in the burner and hence a higher turbine inlet temperature (TIT). Accordingly, the power pro-

duction from the MGT and the electrical efficiency will rise. Furthermore, the pressure ratio (PR) will have an optimum at a relatively low level when introducing a recuperator compared to operation without a recuperator [40]. At high PRs, the temperature of the MGT expander outlet will be lower than the air compressor outlet, neglecting the option of recuperating. The optimum is a result of a trade off between gain in efficiency from exploiting heat in the exhaust gas and loss in efficiency from lowering the PR.

Chapter 4 A ZERO-DIMENSIONAL SOLID OX- IDE FUEL CELL MODEL

To investigate SOFC processes or hybrid systems including SOFCs, as two of the plant configurations presented in the previous chapter, a component model predicting the performance of the SOFCs has been developed. To be able to optimize system parameters, such as operating temperature and pressure, it is necessary to develop an SOFC component model that can predict the SOFC performance depended on its operating conditions. The zero-dimensional component model is added to the existing component library of the simulation tool DNA (Dynamic Network Analysis), which is used in this modelling study. DNA is a simulator made for simulation of mathematical models representing thermodynamic processes. By use of the methodology of network theory in electrical engineering, a procedure for modelling thermodynamic processes is applied. DNA can handle both steady-state and transient process models and has build-in thermodynamic state models of common fluids and solid fuels as well as a component model library. Common equipment, such as heat exchangers, turbomachineries, and burners, is available from the component model library. Furthermore, balancing of energy and mass is done automatically. The FORTRAN-based DNA is free and open source, and more information on DNA can be found in [55], [56], and [57]. The SOFC component model listing can be found in Appendix B.

The developed SOFC submodel calculates the air and fuel outlet compositions and the electrical power production. The calculations are based on the inlet air and fuel compositions and flow rates as well as operating conditions of the SOFC. The operating conditions are partly described by input parameters given directly to the SOFC submodel. These parameters are presented in Table 4.1. The rest comes from system interaction (e.g., operating pressure and inlet temperatures). The SOFC submodel includes an electrochemical model for predicting the electrochemical performance of the SOFC.

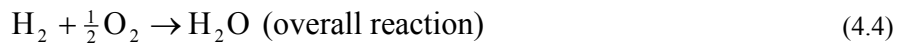
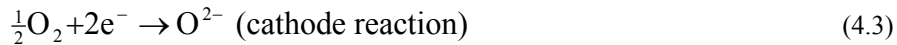
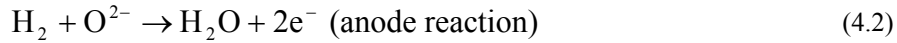
Table 4.1: Direct inputs to the SOFC submodel.

Fuel utilization factor	U_F	0.85
Operating temperature	T_{SOFC}^a	800°C
Anode pressure loss	Δp_a	5 mbar
Cathode pressure loss	Δp_c	10 mbar
Current density	i	300 mA cm ⁻²

^a Equals the SOFC anode and cathode outlet.

In the submodel only H₂ is electrochemically converted in the anode, but the model takes into account that CO produces an extra H₂ molecule through the water-gas-shift (WGS) reaction, while four additional H₂ molecules are produced from CH₄ through internal steam reforming (cf., eq. (2.10)) and WGS of produced CO (cf., eq. (2.5)). Thus, full conversion of CH₄ and CO is assumed. This assumption is fair because the high-temperature and active catalyst containing anode environment ensures (1) fast steam reforming and WGS to reach equilibrium and (2) continuous removal of reforming products via electrochemical reactions [17]. Conversion of NH₃ (cf., eq. (2.11)) is not included in this submodel, thus the total molar flow of H₂ in the anode, after internal steam reforming and WGS, will be as expressed in eq. (4.1).

$$\dot{n}_{\text{H}_2, \text{tot}} = \dot{n}_{\text{H}_2, \text{in}} + \dot{n}_{\text{CO}, \text{in}} + 4\dot{n}_{\text{CH}_4, \text{in}} \quad (4.1)$$



The electrode reactions and the overall fuel cell reaction are as shown in eqs. (4.2) to (4.4). Direct electrochemical conversion of CO (see reaction in Figure 2.5) is neglected because it is most likely that the competing and faster WGS reaction will be the dominant reaction pathway for CO [59]. The amount of hydrogen that is electrochemically converted depends on the fuel utilization factor (U_F), which is defined in eq. (4.5).

$$U_F = \frac{\dot{n}_{\text{H}_2, \text{tot}} - \dot{n}_{\text{H}_2, \text{out}}}{\dot{n}_{\text{H}_2, \text{tot}}} \quad (4.5)$$

The overall fuel cell reaction reveals that the amount of consumed oxygen is half the amount of consumed hydrogen. The cathode outlet composition is

calculated by the following equations; the only species taken into account being O_2 , N_2 , CO_2 , H_2O , and Ar.

$$\dot{n}_{O_2,con} = \frac{U_F \dot{n}_{H_2,tot}}{2} \quad (4.6)$$

$$\dot{n}_{c,out} = \dot{n}_{c,in} - \dot{n}_{O_2,con} \quad (4.7)$$

$$y_{O_2,out} = \frac{\dot{n}_{c,in} y_{O_2,in} - \dot{n}_{O_2,con}}{\dot{n}_{c,out}} \quad (4.8)$$

$$y_{j,out} = \frac{\dot{n}_{c,in} y_{j,in}}{\dot{n}_{c,out}}, \quad j = \{N_2, CO_2, H_2O\} \quad (4.9)$$

$$y_{Ar,out} = 1 - y_{O_2,out} - y_{N_2,out} - y_{CO_2,out} - y_{H_2O,out} \quad (4.10)$$

For the anode flow channel it is assumed that chemical equilibrium is reached at the outlet at the operating temperature and pressure. Chemical equilibrium is characterized by the total Gibbs free energy having its minimum value. With this assumption, the fuel composition leaving the anode can be found by the Gibbs free energy minimization method. This methodology is described in Appendix A and is based on Smith et al. [58] and Elmegaard [56]. In to the Gibbs free energy minimization calculations enters the gas fed to the anode along with the consumed oxygen coming from the cathode (cf., eq. (4.6)). Chemical equilibrium at the anode outlet temperature and pressure is assumed for the following chemical compounds: H_2 , CO , CO_2 , H_2O , CH_4 , and N_2 (Ar is not taken into account).

It is also assumed that the temperature of the solid structure of the SOFC is lumped and equal to the SOFC operating temperature. Furthermore, all gases are considered ideal gases. Finally, it is assumed that the performance of a single SOFC applies for the entire SOFC stack.

Power production from the SOFC depends on the amount of chemical energy fed to the anode and the electrical efficiency of the SOFC (η_{SOFC}) as stated in eq. (4.11). The SOFC efficiency is defined in eq. (4.12) as the product of the reversible efficiency (η_{rev}), the voltage efficiency (η_v), and the fuel utilization factor (U_F) [60].

$$P_{SOFC} = [(\Delta h_f)_{H_2} \dot{n}_{H_2,in} + (\Delta h_f)_{CO} \dot{n}_{CO,in} + (\Delta h_f)_{CH_4} \dot{n}_{CH_4,in}] \eta_{SOFC} \quad (4.11)$$

$$\eta_{\text{SOFC}} = \eta_{\text{rev}} \eta_v U_F \quad (4.12)$$

The reversible efficiency is the maximum possible efficiency defined as the relationship between the maximum available electrical energy (change in Gibbs free energy) and the change in enthalpy of formation, both of which are associated with *full* oxidation of the fuel [60]. This relationship is shown in eq. (4.13).

$$\eta_{\text{rev}} = \frac{(\Delta g_f)_{\text{FO}}}{(\Delta h_f)_{\text{FO}}} \quad (4.13)$$

The expression for the change in Gibbs free energy of formation at full oxidation is shown in eq. (4.14) when considering H_2 , CO , CO_2 , H_2O , CH_4 , and N_2 in the fuel feed. The Gibbs free energies in eq. (4.14) should be determined at the SOFC operating temperature and the partial pressure of the specific reactant or product species. Stoichiometric combustion of the fuel results in a content of CO_2 and H_2O in the product stream as stated in eqs. (4.15) and (4.16). The necessary content of O_2 in the reactant stream for full oxidation to occur can be found in eq. (4.17).

$$\begin{aligned} (\Delta g_f)_{\text{FO}} = & y_{\text{CO}_2, \text{out}, \text{FO}} (g_f)_{\text{CO}_2, \text{p}} + y_{\text{H}_2\text{O}, \text{out}, \text{FO}} (g_f)_{\text{H}_2\text{O}, \text{p}} \\ & - y_{\text{H}_2, \text{in}} (g_f)_{\text{H}_2, \text{r}} - y_{\text{CO}, \text{in}} (g_f)_{\text{CO}, \text{r}} - y_{\text{CH}_4, \text{in}} (g_f)_{\text{CH}_4, \text{r}} \\ & - y_{\text{CO}_2, \text{in}} (g_f)_{\text{CO}_2, \text{r}} - y_{\text{H}_2\text{O}, \text{in}} (g_f)_{\text{H}_2\text{O}, \text{r}} - y_{\text{O}_2, \text{in}, \text{FO}} (g_f)_{\text{O}_2, \text{r}} \end{aligned} \quad (4.14)$$

$$y_{\text{CO}_2, \text{out}, \text{FO}} = y_{\text{CO}, \text{in}} + y_{\text{CH}_4, \text{in}} + y_{\text{CO}_2, \text{in}} \quad (4.15)$$

$$y_{\text{H}_2\text{O}, \text{out}, \text{FO}} = y_{\text{H}_2, \text{in}} + 2y_{\text{CH}_4, \text{in}} + y_{\text{H}_2\text{O}, \text{in}} \quad (4.16)$$

$$y_{\text{O}_2, \text{in}, \text{FO}} = \frac{1}{2} y_{\text{H}_2, \text{in}} + \frac{1}{2} y_{\text{CO}, \text{in}} + 2y_{\text{CH}_4, \text{in}} \quad (4.17)$$

The change in enthalpy of formation is expressed in eq. (4.18), and in this model it is based on LHVs.

$$(\Delta h_f)_{\text{FO}} = (\Delta h_f)_{\text{H}_2} y_{\text{H}_2, \text{in}} + (\Delta h_f)_{\text{CO}} y_{\text{CO}, \text{in}} + (\Delta h_f)_{\text{CH}_4} y_{\text{CH}_4, \text{in}} \quad (4.18)$$

The voltage efficiency (η_v) expresses the electrochemical performance of the SOFC. The calculation of voltage efficiency is described in the following Section.

4.1 ELECTROCHEMICAL MODEL

The electrochemical model is used to calculate the cell potential and voltage efficiency of the SOFC. Both of these values depend on the operating conditions, including temperature, pressure, gas compositions, fuel and oxidant utilization, and load (current density). The operating temperature in Table 4.1 is assumed to be valid for representing the solid temperature of the SOFC in the electrochemical model, and the temperature of the solid structure is denoted T in this description of the electrochemical model. The cell potential and voltage efficiency are defined in eqs. (4.19) and (4.20), respectively.

$$V_{\text{cell}} = E - V_{\text{act}} - V_{\text{ohm}} - V_{\text{conc}} \quad (4.19)$$

$$\eta_v = \frac{V_{\text{cell}}}{E} \quad (4.20)$$

In the following part of the Section, the Nernst potential, or reversible open circuit voltage, (E) and overpotentials are calculated. The total overpotential has contributions from the activation (V_{act}), ohmic (V_{ohm}), and concentration (V_{conc}) overpotentials, which all are described later in this Section.

As a result of the current being drawn from the cell, the partial pressure of both reactants and products change through the cell. Thus, in this study the partial pressure of the j th species is an average across the respective electrode and is here defined as an arithmetic mean between inlet and outlet in eqs. (4.21) and (4.22). The outlet molar fractions are determined by the Gibbs free energy minimization method as described earlier. \bar{p}_a and \bar{p}_c are average partial pressures of the anode and cathode compartment, respectively, taking any pressure losses into account. The average partial pressure of the available hydrogen after internal steam reforming and WGS of CH_4 and CO can be determined from eq. (4.23), equivalent to eq. (4.1), when assuming full conversion of CH_4 and CO to H_2 . The WGS and steam reforming reactions can be found in eqs. (2.5) and (2.10).²

$$\bar{p}_j = \left(\frac{y_{j,\text{out}} + y_{j,\text{in}}}{2} \right) \bar{p}_a, \quad j = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2\} \quad (4.21)$$

$$\bar{p}_{\text{O}_2} = \left(\frac{y_{\text{O}_2,\text{out}} + y_{\text{O}_2,\text{in}}}{2} \right) \bar{p}_c \quad (4.22)$$

² Note, that eq. (4.23) is only valid in water-rich environments. A more generally applicable model is described in Appendix J together with estimates on the error of using eq. (4.23).

$$\bar{p}_{\text{H}_2, \text{tot}} = \bar{p}_{\text{H}_2} + \bar{p}_{\text{CO}} + 4\bar{p}_{\text{CH}_4} \quad (4.23)$$

E can be calculated from the Nernst equation:

$$E = \frac{-\Delta g_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{\bar{p}_{\text{H}_2, \text{tot}} \sqrt{\bar{p}_{\text{O}_2}}}{\bar{p}_{\text{H}_2\text{O}}} \right) \quad (4.24)$$

Because it is assumed that all CO and CH₄ are converted to H₂ before the electrochemical reactions take place, both the change in standard Gibbs free energy (Δg_f^0) and the number of electrons transferred for each molecule of fuel (n_e) are determined for the reaction of H₂ only. Thus, $n_e = 2$ [61] and $\Delta g_f^0 = (g_f^0)_{\text{H}_2\text{O}} - (g_f^0)_{\text{H}_2} - \frac{1}{2}(g_f^0)_{\text{O}_2}$. Note that the standard Gibbs free energy is evaluated at standard pressure, but is still a function of temperature [18].

The activation overpotential is due to an energy barrier (activation energy) that the reacting species must overcome in order to drive the electrochemical reactions. The activation overpotential of each electrode is a non-linear function of the current density and is usually expressed by the Butler-Volmer equation [18] [61] [62] [63] shown in eq. (4.25).

$$i = i_0 \left\{ \exp \left(\alpha \frac{n_e^{\text{BV}} F V_{\text{act}}}{RT} \right) - \exp \left(-(1 - \alpha) \frac{n_e^{\text{BV}} F V_{\text{act}}}{RT} \right) \right\} \quad (4.25)$$

i_0 is the exchange current density, α the charge transfer coefficient, and n_e^{BV} the number of electrons transferred in the single elementary rate-limiting step that the Butler-Volmer equation represents. A value of 0.5 for the charge transfer coefficient is commonly used for fuel cell applications [62], and hereby, the activation overpotential for one electrode can be expressed as in eq. (4.26) as shown by Chan et al. [62]. The value of n_e^{BV} is commonly assumed to be equal to 1 [61].

$$V_{\text{act}} = \frac{2RT}{n_e^{\text{BV}} F} \sinh^{-1} \left(\frac{i}{2i_0} \right) \quad (4.26)$$

The total activation overpotential in this model is hereby defined as the sum of the activation overpotential of each electrode and is based on Chan et al. [62] and Zhu and Kee [61]:

$$\begin{aligned}
 V_{\text{act}} &= V_{\text{act,a}} + V_{\text{act,c}} \\
 &= \frac{2RT}{F} \left[\sinh^{-1} \left(\frac{i + i_n}{2i_{0,a}} \right) + \sinh^{-1} \left(\frac{i + i_n}{2i_{0,c}} \right) \right]
 \end{aligned} \tag{4.27}$$

In this case, an internal current density (i_n) is added to the actual current density in order to account for the mixed potential caused by fuel crossover and electrons passing through the electrolyte. The importance of the internal current density in the case of SOFCs is much less than that for low temperature fuel cells. Thus, the value of i_n is usually very small for SOFCs [17]. In this study, the value of i_n is adjusted when calibrating the electrochemical model. The exchange current density (i_0) is a measure of the level of activity on the electrode at $i=0$ mA cm⁻² and is different for the anode and cathode. Chan et al. [62] use constants to represent both anodic and cathodic exchange current densities, while Zhu and Kee [61] use an expression making the exchange current densities depend on reactant concentrations. Neither of these methods take into account the dependence of temperature that the exchange current densities have. If constant exchange current densities are used, it can be seen from eq. (4.27) that increasing temperature means increasing activation overpotential at the same current density. Thus, increasing temperature will have a negative influence on the SOFC performance, which contradicts with experimental experience. Therefore, to be able to model SOFC performance at various temperatures, the exchange current densities need to depend on temperature. Costamagna et al. [64] studied ways of modelling the exchange current densities from literature, and explicitly tested two empirical models of the anodic exchange current density for Ni/YSZ electrodes with dependence on species concentration and temperature. One is based on results found by Mogensen et al. [65] [66], and this expression is also the one chosen in a later paper by Costamagna et al. [67]. The expression can be found in eq. (4.28) and is also used in this study. The cathodic exchange current density is based on Achenbach [68] and is also used by Costamagna et al. in [64] and [67]. The expression is shown in eq. (4.29). The values of γ and E_{act} can be found in Table 4.2.

$$i_{0,a} = \gamma_a \left(\frac{\bar{p}_{\text{H}_2, \text{tot}}}{\bar{p}_a} \right) \left(\frac{\bar{p}_{\text{H}_2\text{O}}}{\bar{p}_a} \right) \exp \left(\frac{-E_{\text{act,a}}}{RT} \right) \tag{4.28}$$

$$i_{0,c} = \gamma_c \left(\frac{\bar{p}_{\text{O}_2}}{\bar{p}_c} \right)^{0.25} \exp \left(\frac{-E_{\text{act,c}}}{RT} \right) \tag{4.29}$$

The ohmic overpotential is caused by the ohmic resistance towards the oxygen ions passing through the electrolyte and the electrons passing through

the electrodes and interconnects. The ohmic overpotential is dominated by the resistance in the ion conducting electrolyte [61] [62]. According to Braun [69], the ion resistance accounts for 80% of the total ohmic losses. Thus, only the ion resistance through the electrolyte is considered in this model, so the ohmic overpotential is defined as below in eqs. (4.30) to (4.32). The temperature-dependent correlation for the ionic conductivity of the electrolyte (σ_e) is taken from Zhu and Kee [61]. The thickness of the electrolyte (δ_e), the pre-factor ($\sigma_{e,0}$), and activation energy of transport of oxygen ions ($E_{act,e}$) for the calculation of the ionic conductivity of the electrolyte are listed in Table 4.2. $\sigma_{e,0}$ and $E_{act,e}$ are valid for YSZ electrolytes.

$$V_{ohm} = (i + i_n) r_e \quad (4.30)$$

$$r_e = \frac{\delta_e}{\sigma_e} \quad (4.31)$$

$$\sigma_e = \frac{\sigma_{e,0}}{T} \exp\left(-\frac{E_{act,e}}{RT}\right) \quad (4.32)$$

The concentration overpotential is a result of the limitations of diffusive transport of reactants and products between the flow channel and the electrode-electrolyte interface. The effect is increasing with current density, and at a certain current density limit this transport of species is not fast enough to feed the electrochemical reactions taking place, and the partial pressure of reactants at the electrode-electrolyte interface approaches zero. The anode and cathode current density limits are different, and they are dependent on microstructural characteristics of the respective electrode and operating conditions of the SOFC. Detailed models describing this concentration overpotential due to limitation of the diffusive transport are available in the literature (e.g., Zhu and Kee [61], Chan et al. [62], and Kim et al. [70]). For anode supported SOFCs, where the anode layer is much thicker than the cathode layer, the anode limiting current density is much lower than the cathode limiting current density. Thus, the concentration overpotential is dominated by the anode contribution [69] [61]. For reasons of simplification, and since operation at very high current densities are not intended in this study, the anode limiting current density (i_{as}) is assumed to be constant, while the contribution to the concentration overpotential from the cathode is neglected. Also, the cathode concentration overpotential in the model by Chan et al. [62] is infinitesimal. The following expression of the total concentration overpotential is used in this model, and it is based on Kim et al. [70] and Braun [69]:

$$V_{\text{conc}} = -\frac{RT}{n_e F} \left[\ln \left(1 - \frac{i + i_n}{i_{\text{as}}} \right) - \ln \left(1 - \frac{\bar{p}_{\text{H}_2, \text{tot}} (i + i_n)}{\bar{p}_{\text{H}_2\text{O}} i_{\text{as}}} \right) \right] \quad (4.33)$$

The assumed constant anode limiting current density (i_{as}) can be found in Table 4.2. The value of i_{as} is intended to represent SOFC stacks and not single cells because single cells can have much higher limiting current densities.

Table 4.2: Constants in the electrochemical model.

R	8.314 J K ⁻¹ mol ⁻¹	
F	96 485 C mol ⁻¹	
n_e	2	
i_n	6 mA cm ⁻² ^a	
γ_a	5.5×10 ⁹ mA cm ⁻²	[64]
γ_c	7.0×10 ⁸ mA cm ⁻²	[64]
$E_{\text{act},a}$	1.2×10 ⁵ J mol ⁻¹	[64]
$E_{\text{act},c}$	1.2×10 ⁵ J mol ⁻¹	[64]
δ_e	10×10 ⁻⁴ cm	[71]
$E_{\text{act},e}$	0.8×10 ⁵ J mol ⁻¹	[61]
$\sigma_{e,0}$	3.6×10 ⁵ S cm ⁻¹	[61]
i_{as}	1000 mA cm ⁻²	(assumed)

^a Determined by calibration (cf., Section 4.1.1).

So to summarize, the following main equations represent the electrochemical model that predicts the voltage efficiency of the SOFC as a function of species concentration and operating temperature and pressure:

$$\begin{aligned} \eta_v &= \frac{V_{\text{cell}}}{E}, \quad V_{\text{cell}} = E - V_{\text{act}} - V_{\text{ohm}} - V_{\text{conc}} \\ E &= \frac{-\Delta g_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{\bar{p}_{\text{H}_2, \text{tot}} \sqrt{\bar{p}_{\text{O}_2}}}{\bar{p}_{\text{H}_2\text{O}}} \right) \\ V_{\text{act}} &= \frac{2RT}{F} \left[\sinh^{-1} \left(\frac{i + i_n}{2i_{0,a}} \right) + \sinh^{-1} \left(\frac{i + i_n}{2i_{0,c}} \right) \right], \\ i_{0,a} &= \gamma_a \left(\frac{\bar{p}_{\text{H}_2, \text{tot}}}{\bar{p}_a} \right) \left(\frac{\bar{p}_{\text{H}_2\text{O}}}{\bar{p}_a} \right) \exp \left(\frac{-E_{\text{act},a}}{RT} \right) \\ i_{0,c} &= \gamma_c \left(\frac{\bar{p}_{\text{O}_2}}{\bar{p}_c} \right)^{0.25} \exp \left(\frac{-E_{\text{act},c}}{RT} \right) \end{aligned}$$

$$V_{\text{ohm}} = (i + i_n) r_e, \quad r_e = \frac{\delta_e}{\sigma_e}, \quad \sigma_e = \frac{\sigma_{e,0}}{T} \exp\left(-\frac{E_{\text{act},e}}{RT}\right)$$

$$V_{\text{conc}} = -\frac{RT}{n_e F} \left[\ln\left(1 - \frac{i + i_n}{i_{\text{as}}}\right) - \ln\left(1 - \frac{\bar{p}_{\text{H}_2, \text{tot}}(i + i_n)}{\bar{p}_{\text{H}_2\text{O}} i_{\text{as}}}\right) \right]$$

4.1.1 CALIBRATION OF THE ELECTROCHEMICAL MODEL

In the following Section, the electrochemical model of the SOFC is calibrated. Because the model aims to represent the performance of 2nd generation SOFCs from Topsoe Fuel Cell A/S and Risø DTU (National Laboratory for Sustainable Energy), published experimental stack performance data for this SOFC type have been used for calibrating the electrochemical model. These cells are anode supported and the anode consists of Ni/YSZ, the electrolyte of YSZ, and the cathode of LSM/YSZ [20].

The value of the limiting current density, used in the correlation describing the concentration overpotential in eq. (4.33), is assumed because stack performance data at high current densities are not available to the author. A value of 1000 mA cm⁻² is assumed. Of course, this brings some uncertainty into the model at high current densities, but operation in the high current density region is not performed in the conceptual analysis of the studied system scenarios. If this is needed, calibration in the high current density region is recommended.

Concerning the ohmic overpotential, the specific conductivity of the electrolyte, calculated using eq. (4.32), is based on values representing YSZ as published by Zhu and Kee [61]. At 800°C, this results in a specific conductivity of 0.043 S cm⁻¹. An electrolyte thickness of 10 μm – similar to the 2nd generation TOFC/Risø cells, as described by Linderroth et al. [71] – is used to calculate the ohmic resistance.

The open circuit voltage, $V_{\text{cell}}(i=0 \text{ mA cm}^{-2})$, is adjusted by adding an internal current density of 6 mA cm⁻² to the actual current density. Hereby, the overpotentials are not zero at $i=0 \text{ mA cm}^{-2}$, and the open circuit voltage decreases.

The activation overpotential is adjusted to fit the resulting cell potential to the polarization curve published by Linderroth et al. [71]. This is done by applying calibration factors to the exchange current densities. Adjusting the anodic exchange current density by a factor of 2 and the cathodic exchange current density by a factor of 0.5 makes a satisfying fit.

For the data from [71], an active cell area of 81 cm^2 per cell has been assumed. The conditions as stated in [71] are: 75-cell stack ($12 \times 12 \text{ cm}^2$ footprint), 800°C , fuelled with $2000 \text{ Nlitre h}^{-1} \text{ H}_2$ and $1200 \text{ Nlitre h}^{-1} \text{ N}_2$ (which corresponds to $U_F=28\%$ at 18 A or approximately 220 mA cm^{-2} with the assumed active cell area) and $5075 \text{ Nlitre h}^{-1}$ of air. The same conditions are applied in the SOFC component model during calibration. A mix of H_2 and N_2 represents a fuel with both active and inert substances, similar to product gas from gasification. Since the air flow is an input in the SOFC model during calibration, a heat loss/supply is allowed to be able to keep the operating temperature. Both modelled and experimental data as well as the error relative to the experimental data are presented in Figure 4.1. The relative error refers to the right-hand side y-axis. The calibration was done at atmospheric pressure.

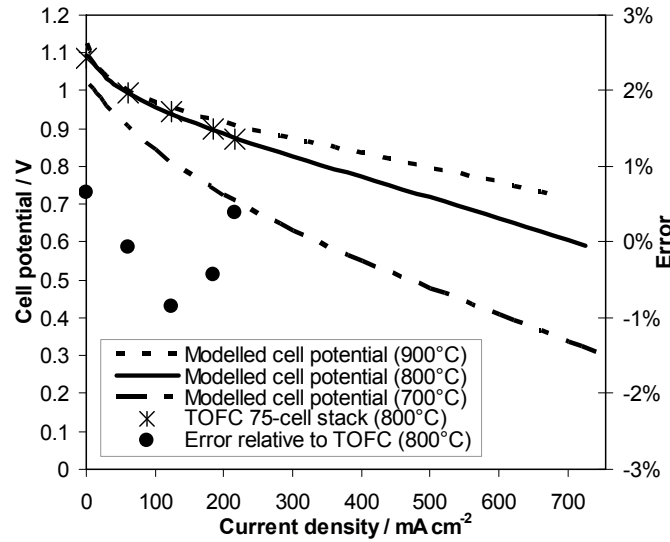


Figure 4.1: Single cell polarization curves based on a 75-cell stack at 800°C and the SOFC model, respectively. The modelled performance is shown for 700, 800, and 900°C , and the relative error between the modelled and experimental performance is shown at 800°C .

The model shows excellent agreement with the experimental data in the region where experimental data are available. The relative error does not exceed $\pm 1\%$. Above $i=220 \text{ mA cm}^{-2}$, the actual TOFC SOFC performance is unknown to the author. As seen in Table 4.1, a current density of 300 mA cm^{-2} was chosen to represent the SOFC load in the following results. Even though 300 mA cm^{-2} is just outside the experimental dataset from [71], it is assumed that the SOFC model represents the TOFC performance to a satisfactory level at this load.

4.2 PARAMETRIC STUDY OF SOFC PERFORMANCE

By varying different operating conditions, the influence of these operating conditions on the performance of the SOFCs is studied. Along with that, the behaviour of the SOFC component model is tested, to see if it acts as expected. The reference conditions in this parametric study are shown in Table 4.3. Some of these conditions are varied one at a time in the following test. Unless otherwise stated, the reference conditions are used. Furthermore it should be noted, that the electric power output is given and kept constant, and that heat losses are neglected. The value of the electric power output is not mentioned because it is not relevant in this parametric study, and since it is kept constant, the fuel flow varies with the SOFC performance. The air flow is controlled by the cooling need of the SOFCs.

Table 4.3: Reference conditions in parametric study.

Fuel	Product gas ^a or 97 vol-% H ₂ + 3 vol-% H ₂ O	
Fuel utilization factor	U_F	0.85
Operating temperature	T_{SOFC} ^b	800°C
Operating pressure	p_{SOFC}	1 bar
Anode temperature difference	ΔT_a	150°C
Cathode temperature difference	ΔT_c	200°C
Anode pressure loss	Δp_a	0 mbar
Cathode pressure loss	Δp_c	0 mbar
Current density	i	300 mA cm ⁻²

^a 26% H₂, 30% N₂, 18% CO, 12% CO₂, 13% H₂O, and 1% CH₄ by volume.

^b Equals the SOFC anode and cathode outlet.

First, the influence of current density on the different overpotentials are examined and depicted using product gas similar to that from the Viking gasifier, Figure 4.2, and using hydrogen with 3 vol-% of water, Figure 4.3, as fuels. Also the resulting cell potential and power density is plotted. The dominant polarization loss is the activation overpotential for both fuels, but the concentration overpotential also has great influence when approaching the limiting current density of 1000 mA cm⁻². On the contrary, the ohmic overpotential is relatively low, though increasing with current density as for all three overpotentials. The modelled polarization curve and corresponding overpotentials cannot be directly compared to general results from literature because it is calibrated specifically to one TOFC stack. Though, the sizes of the three overpotentials – relative to each other – seem reasonable when compared to the model by Chan et al. for anode supported SOFCs operated at 800°C, at atmospheric pressure, and with hydrogen (fig. 6 in [62]); activation overpotential being the highest, ohmic polarization the lowest, and the losses from gas diffusion limitations in between. Better performance is ob-

tained when using almost pure hydrogen compared to the more dilute product gas. This is due to lower activation overpotential, while the Nernst potential, ohmic losses, and concentration losses seem unaffected by the fuel choice. The average partial pressure of hydrogen after internal steam reforming and WGS ($\bar{p}_{\text{H}_2, \text{tot}}$), eq. (4.23), is approximately 0.56 bar and 0.28 bar when fuelled with hydrogen and product gas, respectively. The reason is

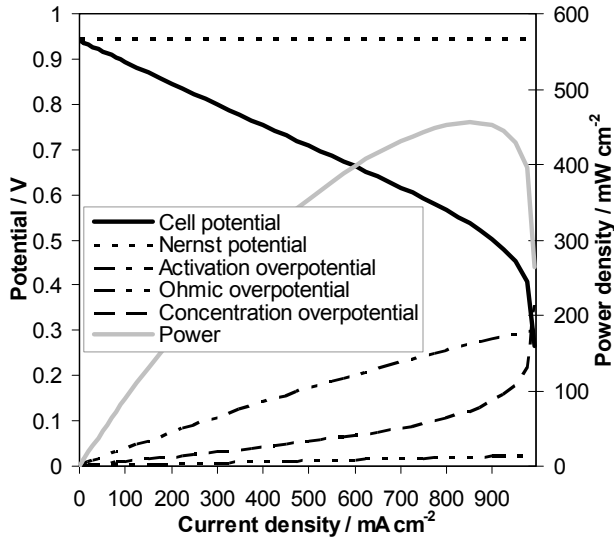


Figure 4.2: Nernst potential, polarization losses and resulting single cell potential and power density as a function of current density, when operating on product gas.

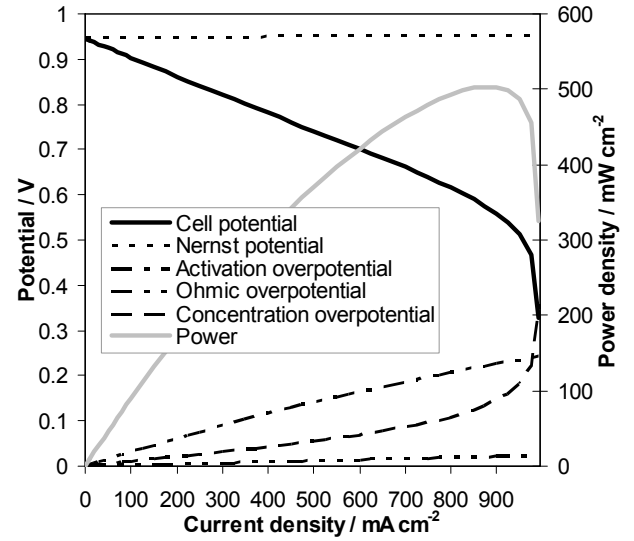


Figure 4.3: Nernst potential, polarization losses and resulting single cell potential and power density as a function of current density, when operating on hydrogen with 3 vol-% of water.

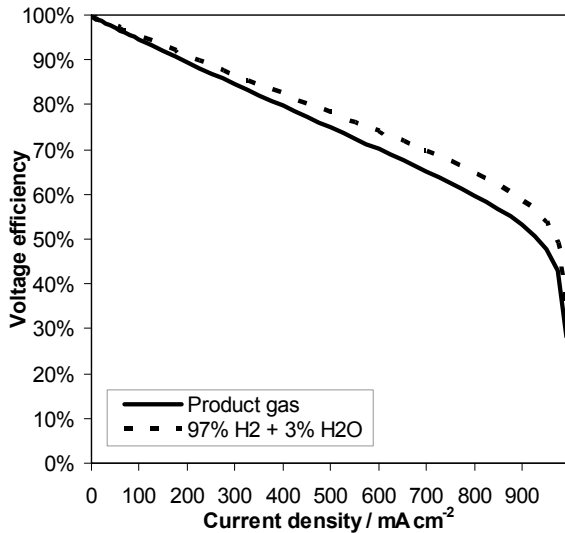


Figure 4.4: Voltage efficiency as a function of current density for two different fuels.

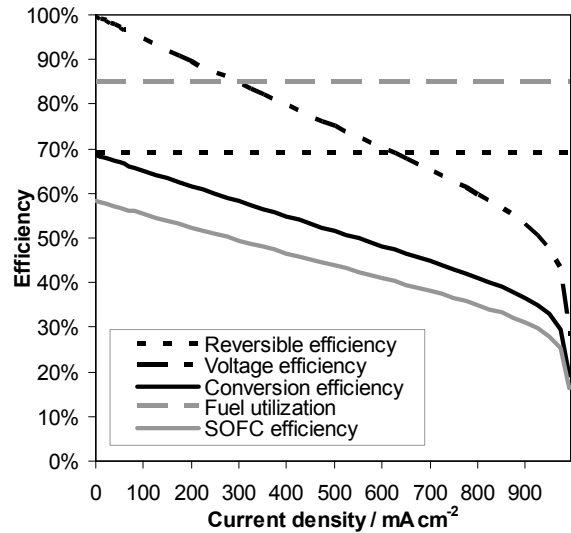


Figure 4.5: Fuel cell efficiencies as a function of current density using product gas.

the inert parts (mainly N_2) in the product gas. Offhand, this should explain the better performance using almost pure hydrogen as fuel. Examining the expressions used in the electrochemical model, it is found that the Nernst potential, eq. (4.24), and the concentration overpotential, eq. (4.33), more exactly are depended on the ratio between $\bar{p}_{H_2, \text{tot}}$ and \bar{p}_{H_2O} , when only varying the fuel composition - \bar{p}_{O_2} is constantly close to $p_{O_2, \text{in}}$ because a high excess flow of air is used to cool the SOFCs. Since \bar{p}_{H_2O} is approximately 0.44 bar and 0.24 bar with hydrogen and product gas, respectively, the ratios between $\bar{p}_{H_2, \text{tot}}$ and \bar{p}_{H_2O} are almost the same with the two fuels (1.26 and 1.14, respectively). Thus, the Nernst potential and concentration overpotential are similar with the two fuels, along with the ohmic overpotential, which is not affected by fuel choice. This leaves only the activation overpotential to be significantly depended on fuel choice, which also can be seen by examining the anodic exchange current density expression, eq. (4.28). In this expression, the anodic exchange current density is depended on the product of, rather than the ratio between, $\bar{p}_{H_2, \text{tot}}$ and \bar{p}_{H_2O} . This product is higher when using hydrogen (0.25 versus 0.07), resulting in a higher anodic exchange current density and, thereby, a lower activation overpotential. In reality, the Nernst potential and concentration overpotential can be affected by fuel choice because using eq. (4.23) ($\bar{p}_{H_2, \text{tot}}$) is not always valid (cf., Appendix J).

In Figure 4.4, the voltage efficiencies, defined in eq. (4.20), resulting from the ratio between the cell potential and the Nernst potential from Figure 4.2 and Figure 4.3, are shown for easy comparison between the two fuel types. Voltage efficiencies are measures of the electrochemical performance of the SOFC. The different fuel cell efficiencies using product gas are depicted in Figure 4.5 as a function of current density. The reversible efficiency, defined in eq. (4.13), is not affected by the load, whereas the voltage efficiency is sensible to the chosen current density because it is proportional to the cell potential. A conversion efficiency is here defined as the product of the reversible efficiency and the voltage efficiency (cf., eq. (4.34)). This conversion efficiency describes how well the *reacting* fuel is converted to electricity, without taking the loss of excess fuel into account. From a system point of view, the conversion efficiency, as it is defined here, can give a better view on the performance of the SOFC when combined with other thermal cycles, e.g., a Brayton cycle. In hybrid systems, excess fuel from the SOFC can be utilized elsewhere and is not necessarily a loss. The fuel utilization might even be kept low to satisfy other parts of the hybrid system than the SOFC.

$$\eta_{\text{conv}} = \eta_{\text{rev}} \eta_v \quad (4.34)$$

By including the fuel utilization factor, the overall SOFC efficiency is obtained. At $i=300 \text{ mA cm}^{-2}$, the overall SOFC efficiency from added fuel to electricity is 49%, while the voltage efficiency and conversion efficiency is 85% and 58%, respectively.

As for the study on influence of current density on overpotentials, resulting cell potential and power density as well as the associated efficiencies, the

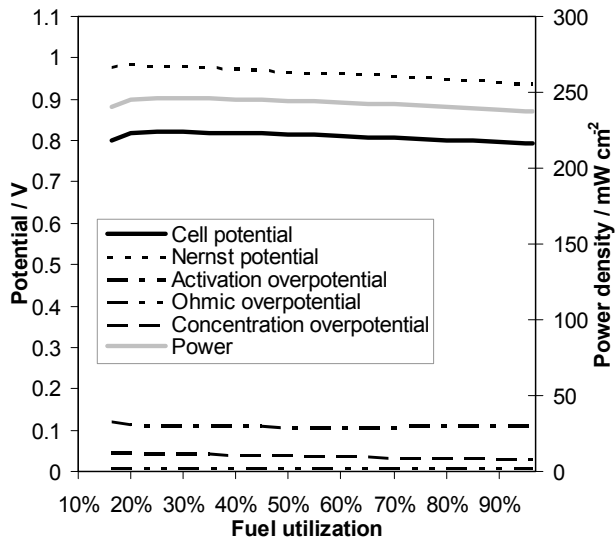


Figure 4.6: Nernst potential, polarization losses, and resulting single cell potential and power density as a function of fuel utilization, when operating on product gas.

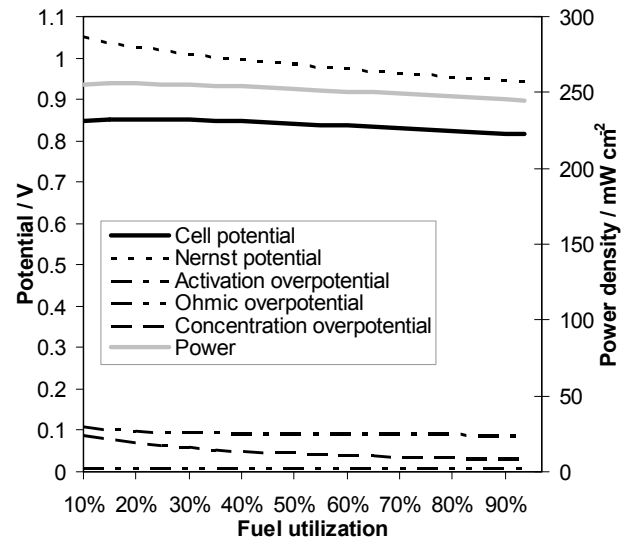


Figure 4.7: Nernst potential, polarization losses, and resulting single cell potential and power density as a function of fuel utilization, when operating on hydrogen with 3 vol-% of water.

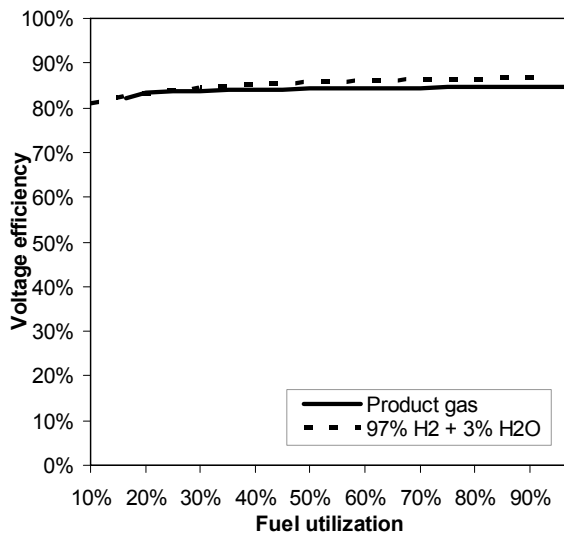


Figure 4.8: Voltage efficiency as a function of fuel utilization for two different fuels.

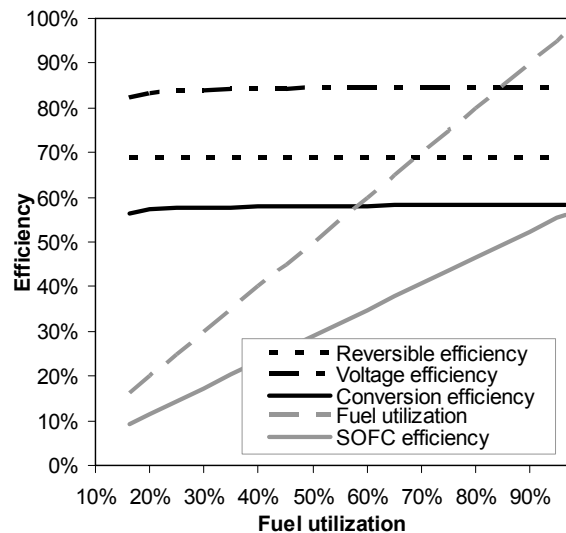


Figure 4.9: Fuel cell efficiencies as a function of fuel utilization using product gas.

following description looks at varying fuel utilization. The reference value of U_F is 85%. When the fuel utilization factor is increased, less unreacted fuel leaves the anode compartment. Thus, the average partial pressure of available hydrogen is reduced and the average partial pressure of water is increased. This explains the decreasing tendency of the Nernst potential with increasing fuel utilization in Figure 4.6 and Figure 4.7. Still, the average partial pressure of oxygen in the cathode flow channel is not changing significantly in most of the fuel utilization range because the excess air flow is very high. Though, at very low fuel utilization, the air flow reduces notably, because the higher fuel flow delivers significant cooling of the SOFC (the air flow is calculated based on the cooling need to maintain the operating temperature). Hereby, the average oxygen partial pressure decreases along with the Nernst potential. Considering the case when fuelling with product gas, the mass flow of air fed to the cathode at $U_F=16\%$ is reduced to 17% of the corresponding flow when operating at $U_F=85\%$. This phenomenon ensures the presence of an optimum in the resulting cell potential, which can be seen in Figure 4.6 at approximately 25% fuel utilization. In Figure 4.7, the influence from reducing air flow cannot be seen, since the air mass flow at $U_F=16\%$ is only reduced to 85% of the corresponding flow at $U_F=85\%$. Thus, the average partial pressure of oxygen is not notably affected, thereby not decreasing the Nernst potential. Still, the resulting cell potential has an optimum around $U_F=20\%$, but this appears to be due to increased anodic concentration overpotential at low fuel utilization when fuelled by hydrogen with 3 vol-% of water. From eq. (4.33), describing the concentration overpotential, it is evident that the concentration overpotential is only governed by the ratio between $\bar{p}_{H_2,tot}$ and \bar{p}_{H_2O} when changing the fuel utilization. In the case of using hydrogen with 3 vol-% of water, this ratio increases more when lowering the fuel utilization factor than in the case using product gas (at $U_F=85\%$, the ratios between $\bar{p}_{H_2,tot}$ and \bar{p}_{H_2O} are 1.3 and 1.1 for hydrogen and product gas, respectively, while at $U_F=16\%$, the ratios are 8.1 and 3.0, respectively). This explains the more pronounced increase in the concentration overpotential when decreasing the fuel utilization in the case of using almost pure hydrogen versus using product gas.

The voltage efficiencies at varying fuel utilization, when using either hydrogen or product gas, are compared in Figure 4.8. The electrochemical performance when fuelled by humidified hydrogen is slightly higher when the fuel utilization is above 30%. In Figure 4.9, the reversible efficiency, when fuelled by product gas, is constantly 69% no matter the chosen fuel utilization. The reversible efficiency is only depended on the fuel composition at inlet as well as the operating temperature and pressure. The voltage efficiency is not very sensitive to the fuel utilization, and similar for the conversion efficiency. From this, it can be concluded that the *reacting* product gas

in the SOFC is converted almost equally efficient above $U_F=25\%$. The picture changes radically, if the loss of excess fuel is taken into account. If so, the fuel utilization should be maintained at a high level. The importance of utilizing all the fuel is evident, but can also be done downstream the SOFC.

The performance of SOFCs depends significantly on the chosen operating temperature as illustrated in Figure 4.10 to Figure 4.13. Decreasing the tem-

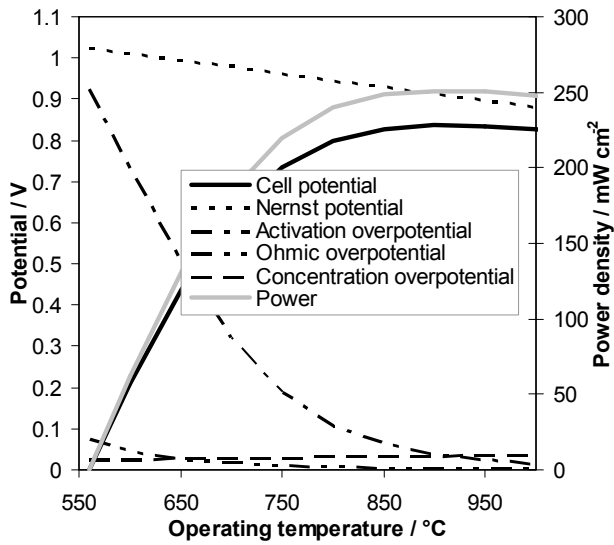


Figure 4.10: Nernst potential, polarization losses, and resulting single cell potential and power density as a function of operating temperature, when operating on product gas.

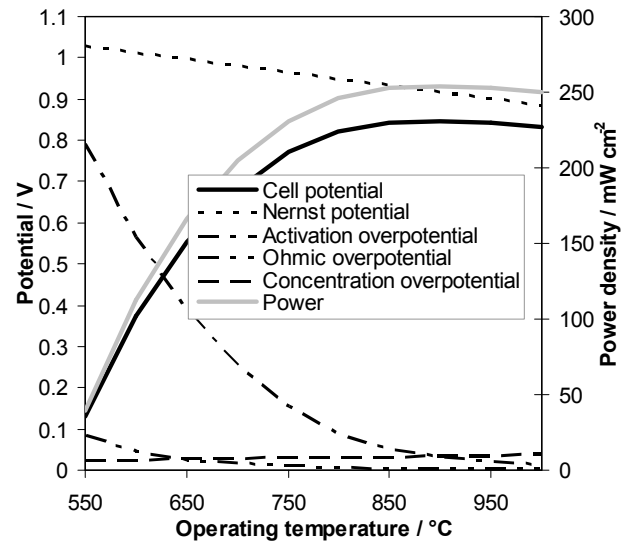


Figure 4.11: Nernst potential, polarization losses, and resulting single cell potential and power density as a function of operating temperature, when operating on hydrogen with 3 vol-% of water.

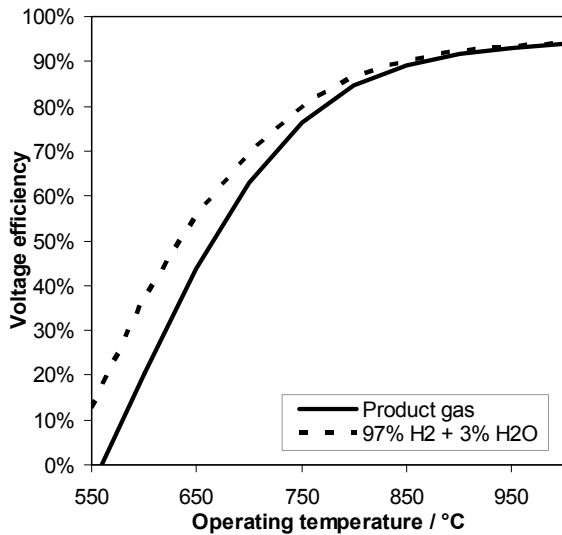


Figure 4.12: Voltage efficiency as a function of operating temperature for two different fuels.

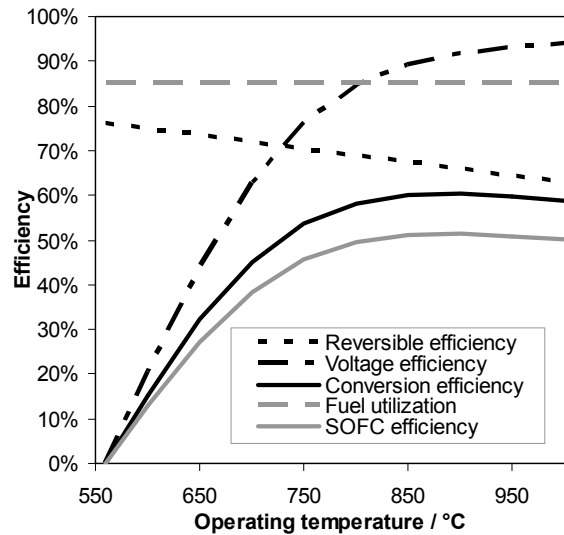


Figure 4.13: Fuel cell efficiencies as a function of operating temperature using product gas.

perature from the reference value of 800°C severely degrades the performance no matter the chosen fuel. From Figure 4.10 and Figure 4.11, it is obvious that the major contributor to the performance trend is the activation overpotential. Lowering the temperature increases the activation overpotential dramatically. From eq. (4.27), it seems that the activation overpotential should increase with increasing temperature, but the exchange current densities, eqs. (4.28) and (4.29), ensure the opposite trend. This underlines the importance of using temperature depended exchange current densities in the model, and not constants, if the model should be able to predict the performance at various temperature levels. At lower temperature, the ionic conductivity of the electrolyte (σ_e), eq. (4.32), decreases causing the ohmic overpotential to increase. The concentration overpotential, on the other hand, is directly proportional to the temperature, as seen in eq. (4.33), so the losses from limited gas diffusion increases with rising temperature, though very moderately. The Nernst potential, eq. (4.24), shows a decreasing trend at rising temperature, which dominates and causes the resulting cell potential to drop, when the temperature is above 900°C.

Considering both fuels in Figure 4.12, it can be concluded, that the electrochemical performance increase with rising temperature in all of the shown temperature range. Contrary for product gas in Figure 4.13, the reversible efficiency, eq. (4.13), decrease with increasing temperature causing the conversion efficiency, eq. (4.34), and the overall SOFC efficiency, eq. (4.12), to peak around 900°C at approximately 60% and 51%, respectively. The decreasing tendency of the reversible efficiency at rising temperature is due to the lower change in the Gibbs free energy of formation (cf., eq. (4.14)) at higher temperature.

The influence of operating pressure is depicted in Figure 4.14 to Figure 4.17. None of the overpotentials are depended on the operating pressure. The only parameters, included in the expressions describing the overpotentials, which are depended on pressure, are either ratios between partial pressures or ratios between partial pressure and absolute pressure, the latter being equal to the molar fraction. On the other hand, the Nernst potential, eq. (4.24), increases with growing pressure, improving the resulting cell potential. The increasing tendency with growing pressure in eq. (4.24) only originates from the increasing oxygen partial pressure because the increasing partial pressure of hydrogen and water counterbalance each other.

The voltage efficiencies for the two studied fuel types are rather constant with varying pressure as depicted in Figure 4.16. Increasing the operating pressure from 1 to 20 bar improves the voltage efficiency from 84.5% to 85.6% in the case of running on product gas and from 86.5% to 87.4% running on hydrogen. The reversible efficiency, eq. (4.13), in Figure 4.17

shows an increasing trend with growing pressure. This is a result of an increase in the change in Gibbs free energy of formation (cf., eq. (4.14)), which is evaluated at the partial pressure of the specific reactant or product species. Hereby, the resulting SOFC efficiency shows a moderate sensitivity to the chosen operating pressure. The performance gain from increasing the pressure is greatest in the low pressure region near, atmospheric conditions, expressed by the higher slope.

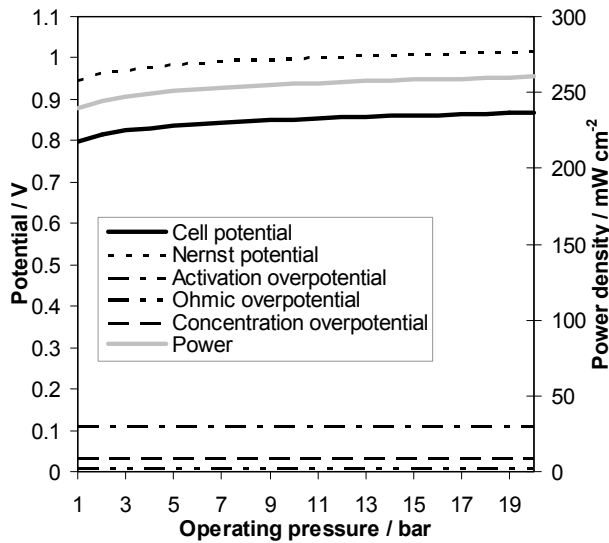


Figure 4.14: Nernst potential, polarization losses, and resulting single cell potential and power density as a function of operating pressure, when operating on product gas.

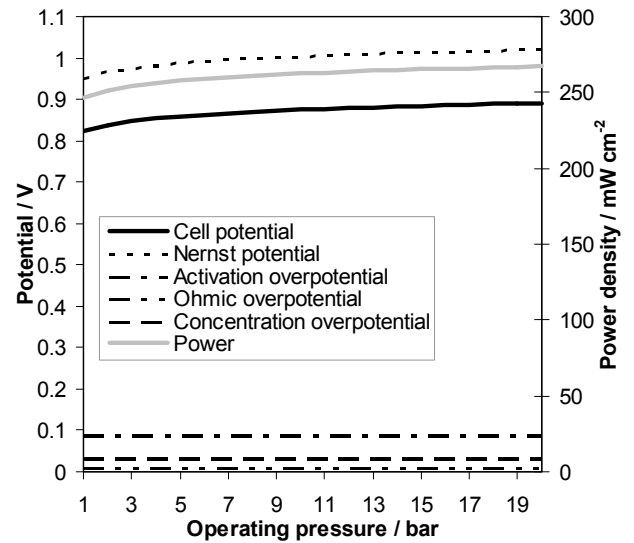


Figure 4.15: Nernst potential, polarization losses, and resulting single cell potential and power density as a function of operating pressure, when operating on hydrogen with 3 vol-% of water.

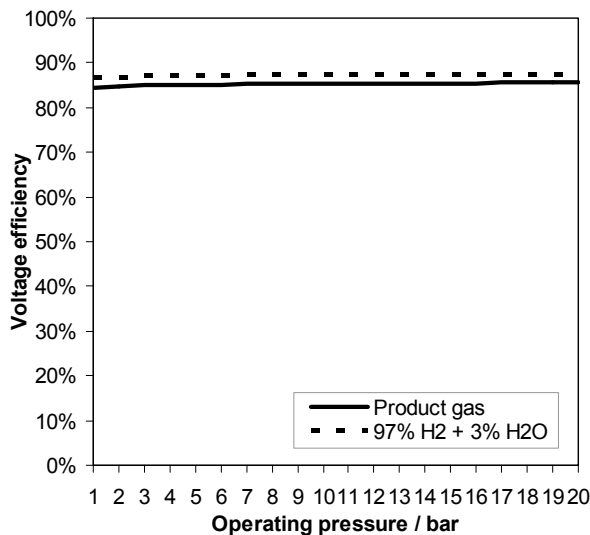


Figure 4.16: Voltage efficiency as a function of operating temperature for two different fuels.

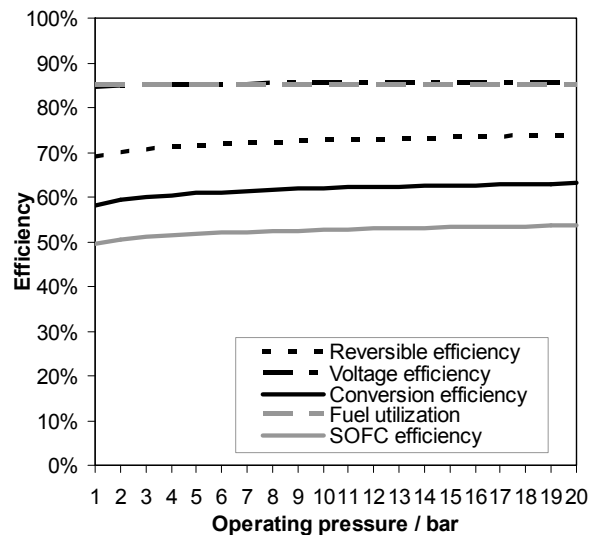


Figure 4.17: Fuel cell efficiencies as a function of operating temperature using product gas.

4.3 SUMMARY

An SOFC component model has been developed for use in process simulations. The component model is zero-dimensional, but still predicts the electrical power production of SOFCs at various operating conditions and fuel types. This is convenient when optimizing important system parameters.

Calibration of the SOFC component model was performed against literature, with the aim of representing the SOFC performance of 2nd generation SOFCs from Topsoe Fuel Cell A/S and Risø DTU (National Laboratory for Sustainable Energy).

The SOFC component model can also be used to evaluate the influence of operating conditions on the SOFC performance. This was examined in the parametric study. The SOFC performance showed to be highly sensitive to the selected current density (cf., Figure 4.5 when fuelled by product gas). Higher current density reduces the SOFC efficiency. The electrical power production increases with increasing current density, though, until closing in on the limiting current density. From an energy efficiency viewpoint, the current density should be as low as possible, but to produce a specified amount of electrical power, lowering the current density will increase the investment costs. Thus, from an economical viewpoint, an optimal current density exists at a higher level compared to that of an energy efficiency viewpoint. Varying the fuel utilization factor greatly impacts the resulting SOFC efficiency, and Figure 4.9 implies that the fuel utilization should be maintained at a high level. Still, the electrochemical performance is rather insensitive to the chosen fuel utilization in most of the studied range of fuel utilization. At very low fuel utilization, the fuel flow becomes high enough to cool the SOFC significantly. Thus, a limited air flow can reduce the SOFC performance because the air flow is calculated based on the cooling need. Also, the efficiency from producing electricity from the *reacting* fuel in the SOFC is almost constant. Hereby, the fuel utilization can be changed, for reasons originating in the rest of the system, without decreasing or increasing how efficiently the reacting fuel in the SOFC is converted to electricity. The influence of temperature on the SOFC performance is severe. The electrochemical performance increases with temperature (cf., Figure 4.13 for the case of product gas), but the overall SOFC efficiency reaches a peak at high temperature due to the decreasing reversible efficiency. It should be noted, that the model is not validated in all of the temperature range shown in Figure 4.13, but only at 800°C. The whole range is included to ease the understanding of the reasons to the temperature dependency of the SOFC performance. The sensitivity of the SOFC performance to the chosen operating pressure is only moderate. The SOFC efficiency shows an increasing trend with increasing pressure, but highest impact of increasing

pressure is obtained just above atmospheric pressure, while less impact shows at higher pressures. Thus, the operating pressure does not necessarily need to be maximized.

The parametric study shows that the SOFC performance predicted by the SOFC component model is depended on the different operating conditions. The described dependencies can also be used as guidelines for optimal SOFC operation. The component model is accepted for further use in the coming system-level models.

Chapter 5 DEVELOPMENT OF THE PROCESS MODELS

Mathematical models describing the thermodynamic processes of the three studied scenarios have been developed to be able to investigate their steady-state performances. The models rely on connecting zero-dimensional component models to generate complete system-level models. As mentioned in the introduction to Chapter 4, the simulation tool used in this modelling study is DNA (Dynamic Network Analysis), which is made for simulations of mathematical models representing thermodynamic processes. Plant model listings can be found in Appendix C, Appendix D, and Appendix E.

Minor adjustments in the system layouts are made for the mathematical models compared to the chosen systems presented in Chapter 3, Figure 3.1. These can be seen in Figure 5.1 and are; mixing of dryer steam and preheated air before introduction to the gasification reactor, and removal of all impurities in a gas cleaning unit instead of only particulates in a bag filter. The reason for mixing preheated air and dryer steam is that the gasifier component model is defined in such a way that the solid feedstock enters separately from gases. Since it is assumed that the product gas after particulate removal is clean enough in this study, and that the impact of remaining impurities are neglected, a simple gas cleaning component model removing all impurities is used. Not illustrated is an inverter, converting the SOFC electric power production from DC to AC, as well as a generator situated on the shaft of the gas turbine producing the net electric MGT power. In the SOFC configuration (without a MGT), the product gas and air blowers are driven by an electric motor. Furthermore, it is assumed that heat losses from components (except the inverter and generator) and pipework are neglected, and that carbon deposition will not occur in any components.

The stated temperatures in Figure 5.1 are the chosen temperature conditions for the studied scenarios. Some of the values are given in the component

models, and the rest can be found in Table 5.1 that contains the system-level inputs. 15°C and atmospheric pressure are the ambient conditions, and regarding pressures in the system, these are defined in some components and calculated from stated pressure drops elsewhere.

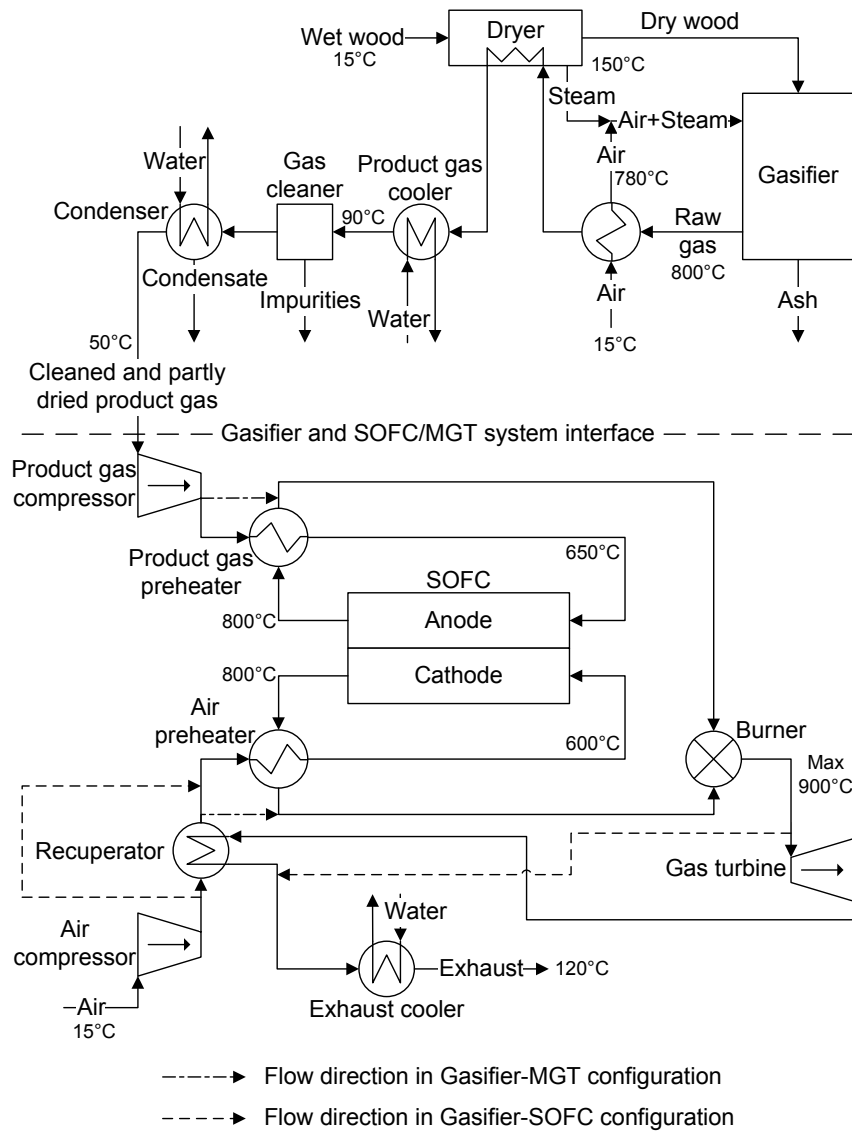


Figure 5.1: Flow sheet of modelled scenarios with specified temperature conditions.

The raw gas temperature of 800°C coming out of the gasification reactor is defined in the gasifier component model, and likewise for the SOFC electrode outlets, the off gas temperatures of 800°C are defined in the SOFC component model. The preheated air for the gasifier (780°C), the preheated product gas (650°C), the preheated air for the SOFC (600°C), and the exhaust gas temperature (120°C) are all defined indirectly by introducing a

pinch point temperature difference in the heat exchanger component models (cf., Table 5.7). The gas cleaning temperature (90°C) and temperature of the cleaned and partly dried product gas leaving the gasification plant (50°C) are equal to those of the Viking demonstration plant.

The mass flow of air fed to the SOFC cathode is calculated based on the cooling need of the SOFC to be able to keep its operating temperature. The pressure on the cathode side is derived from the anode side through the burner submodel, which sets the pressure of fuel and oxidant feed to be equal.

Table 5.1: System-level inputs.

Media	$T / ^\circ\text{C}$	p / bar	$\dot{m} / \text{kg h}^{-1}$
Wet wood	15	1.013	154.8 ^a
Dry wood	150		
Ambient air (gasifier)	15		
Ash		1.013	
Cooled product gas	90		
Cleaned and partly dried product gas	50		
Burner fuel inlet / preheated product gas (anode inlet)		Varied ^b	
Ambient air (SOFC/MGT)	15	1.013	
Exhaust		1.013	

^a Corresponds to a thermal input of 499.2 kW_{th} (LHV).

^b Defined in the burner inlet in the MGT scenario, the anode inlet in the SOFC-MGT scenario, and is not an input in the SOFC configuration.

Table 5.2: Solid biomass data.

Ultimate analysis / wt-% (dry)		
C	48.8	[11]
H	6.2	[11]
O	43.9	[11]
S	0.02	[11]
N	0.17	[11]
Ash	0.91	[11]
Properties		
LHV	18.28 MJ kg ⁻¹ (dry)	[11]
c _p	1.35 kJ kg ⁻¹ K ⁻¹	
x _{H2O}	32.2 wt-%	[11]

Table 5.3: Air composition, predefined in DNA.

Compound	Molar fraction / vol-%
N ₂	77.29
O ₂	20.75
H ₂ O	1.01
Ar	0.92
CO ₂	0.03

The input media to the process is solid biomass and air, and these are specified in Table 5.2 and Table 5.3, respectively. The solid biomass used in this

work is the same as used in the Viking gasifier as published by Ahrenfeldt et al. [11]. The biomass feedstock is added as woodchips of primarily beech with small amounts of oak [11]. The small amount of chlorine documented in [11] is not included in the solid biomass in this study. Anyway, the main part of the chlorine in the biomass published by Ahrenfeldt et al. [11] originates from spraying the wood with seawater to avoid it from drying up when stored and not from the biomass source itself.

All the inputs to the system-level models can be found by collecting data from Table 4.1, Table 4.2, Table 5.1, Table 5.2, Table 5.3, Table 5.4, Table 5.6, and Table 5.7.

5.1 SUBMODELS

Connecting submodels of the different components constitute the total process model. In the following, documentations of the employed component models are presented. Main components in the total process are the gasifier and the SOFC, while components like heat exchangers are considered peripheral. The MGT consists of several components, but these are described together in one Section below because the MGT components are considered as connected in one main technology of the total process. The SOFC component model is described in detail in Chapter 4, therefore not described here. Direct input parameters stated in the component model descriptions below are user defined inputs. In addition to these, the submodels get inputs from their connections to the rest of the system. These can be user defined from a system level (Table 5.1) or outputs from other component models.

5.1.1 GASIFIER

The gasifier component model calculates the product gas composition and the produced ashes based on the inlet media compositions and the operating conditions. The input parameters defining the operating conditions in the gasifier submodel are given in Table 5.4. The gasifier pressure loss is defined as the difference between the inlet air and steam mixture and the outlet product gas.

Table 5.4: Direct inputs to the gasifier submodel.

Operating pressure	p_{gasifier}^a	0.998 bar
Operating temperature	T_{gasifier}^a	800°C
Pressure loss	$\Delta p_{\text{gasifier}}$	5 mbar
Carbon conversion factor	CC	1
Additional non-equilibrium methane in product gas	$METH$	0.01 vol-% ^b

^a Equals the gasifier outlet.

^b Determined by calibration (cf., Section 5.1.1.1).

In the gasifier, the incoming flows are converted into product gas and ashes. The ashes are represented by SiO_2 and unconverted carbon. SiO_2 originates from a defined content in the inlet biomass, while the unconverted carbon is controlled by a defined carbon conversion factor (CC). The amount and composition of ashes are calculated by eqs. (5.1), (5.2), and (5.3).

$$\dot{m}_{\text{ash,out}} = \dot{m}_{\text{wood,in}} [x_{\text{SiO}_2,\text{in}} + x_{\text{C,in}} (1 - CC)] \quad (5.1)$$

$$x_{\text{SiO}_2,\text{out}} = \frac{\dot{m}_{\text{wood,in}} x_{\text{SiO}_2,\text{in}}}{\dot{m}_{\text{ash,out}}} \quad (5.2)$$

$$x_{\text{C,out}} = 1 - x_{\text{SiO}_2,\text{out}} \quad (5.3)$$

As for the SOFC submodel, it is assumed that chemical equilibrium is reached at outlet at the operating temperature and pressure, so the Gibbs free energy minimization method is applied (cf., Appendix A). The product gas from the gasifier model can consist of the following chemical compounds at equilibrium: H_2 , N_2 , CO , CO_2 , H_2O , CH_4 , H_2S , and Ar .

An option for adjusting the methane content in the product gas is included in order to reach product gas compositions, which contain more methane than in the corresponding composition at equilibrium. Thus, the product gas composition can be adjusted to match realistic gas compositions, e.g., from the Viking gasifier. The input parameter *METH* is used for this adjustment and is defined as the amount of additional methane in the product gas that does not originate from the equilibrium calculations.

5.1.1.1 GASIFICATION PROCESS CALIBRATION

In the following Section, the gasification process is calibrated. To calibrate the gasification process modelled here, all of the modelled gasification plant, from the biomass feedstock to the cleaned and dried product gas, is compared to the complete Viking gasifier plant. Both the test data from the Viking gasifier and calculated data from the gasifier model are based on a biomass feedstock as reported by Ahrenfeldt et al. [11] and described in Table 5.2. In the gasifier model, the parameter *METH* is adjusted to achieve an acceptable CH_4 content in the product gas. By setting *METH* equal to 0.01 vol-% (as shown in Table 5.4), the calculated dry gas composition becomes similar to that of the Viking gasifier. As seen in Figure 5.2 and Table 5.5, the produced gas composition and the LHV from the gasifier model are close to the Viking data. The CO_2 content shows the greatest deviation, whereas the resulting LHVs are similar. The overall performance of the

modelled gasifier is also similar to that of the Viking gasifier, as indicated by the cold gas efficiencies (defined in eq. (2.8)).

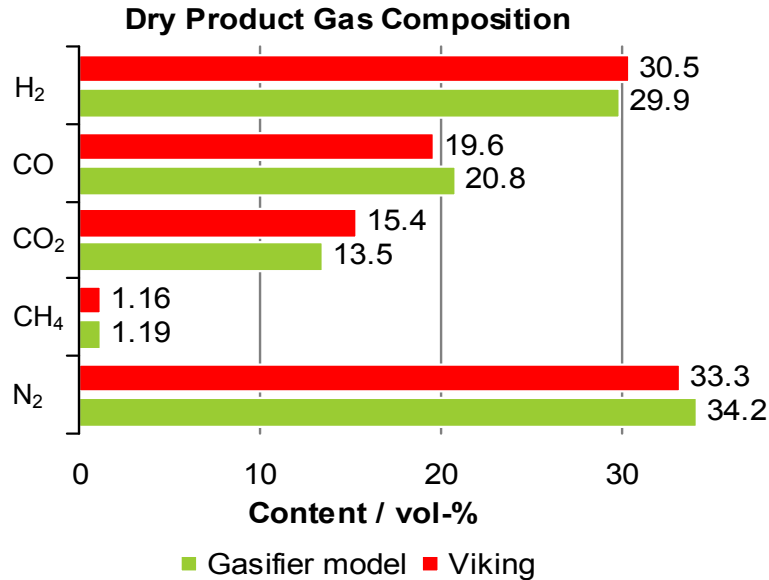


Figure 5.2: Comparison of dry product gas composition from the gasifier model with experimental data [11] from the Viking gasifier.

Table 5.5: LHV and cold gas efficiency of the gasifier model and the Viking gasifier.

	Gasifier model	Viking gasifier [11]
LHV (MJ kg ⁻¹)	6.3	6.2
Cold gas efficiency	94%	93%

5.1.2 MICRO GAS TURBINE

Modelling of gas turbines is well described in the open literature. The reader is referred to Saravanamuttoo et al. [40] for details. Characteristics of the turbomachinery and other components connected to the MGT are listed in Table 5.6. The MGT components are only used in the MGT and SOFC-MGT configurations. In the SOFC case, fuel and air blowers are used instead of compressors, and these are driven by electric motors. Inputs related to the components in the SOFC configuration can be found in the next Section describing peripheral equipment.

Table 5.6: Inputs related to the MGT components.

	Isentropic eff. / %	Mechanical eff. / %	
Fuel and air compressor ^a	75	98	
	Isentropic eff. / %	TIT / °C	
Gas turbine expander ^a	84	900 ^b	
	Δp		
Burner	0.6‰ ^c		
	$\Delta p_{\text{hot side}} / \text{mbar}$	$\Delta p_{\text{cold side}} / \text{mbar}$	$\varepsilon / \%$
Recuperator ^a	10	10	85
	Efficiency / %		
Generator ^a	95		

^a Only used in the MGT and SOFC-MGT configurations.

^b Only an input in the MGT configuration.

^c 0.6‰ equals 1.5 mbar if 2.5 bar is present at the inlet.

The air and product gas compressor submodels calculate the mechanical power required to increase the pressure of the working fluid. This is done based on specified isentropic and mechanical efficiencies. The gas turbine submodel works in the same manner as the compressor submodels, except that no mechanical losses are taken into account. The turbine inlet temperature is limited to 900°C in the Gasifier-MGT case, while it varies in the SOFC-MGT arrangement. The performances of the compressors and MGT expander correspond to common performance data for a MGT of this scale, e.g., see [44], but it should be noted that the operating conditions are non-conventional due to a low turbine inlet temperature in the SOFC-MGT case and a low heating value of the fuel gas in all cases. The outlet pressure from the MGT expander depends on the total pressure loss downstream the MGT, because of the plant exhaust pressure, which is fixed at 1.013 bar. Because of the pressure drop in the recuperator and exhaust cooler, the outlet pressure from the MGT expander is slightly higher (1.033 bar). Constant heat exchanger effectiveness is applied to the recuperator to ensure realistic performance.

5.1.3 PERIPHERAL EQUIPMENT

Besides the gasifier and SOFC component models, modelling the rest of the components are mostly standard. These are therefore not described in detail, but are briefly discussed below. Furthermore, the peripheral equipment component models are not considered for validation or calibration.

The biomass dryer reduces the water content in the biomass from 32.2 wt-% to 5 wt-% by heating it to 150°C. During the drying process in the Viking

gasifier, the hot product gas directly heats the biomass in a stream separated dryer. Contrary, the upscaled two-stage gasification process (cf., Figure 2.3) uses steam drying by heating a steam loop. In the latter case, the steam is in direct contact with the biomass. The modelling of the drying process is done by introducing a steam loop to transfer the heat from the product gas to the biomass as illustrated in Figure 5.3. The superheated steam dries the biomass, and the moisture from the biomass leaves the dryer together with the hot steam. The excess steam is separated from the steam loop and is exactly equal to the amount that evaporates from the biomass. To model a stream separated dryer as in the Viking gasifier, pressure and heat losses in the steam loop are set equal to zero and the steam blower is assumed to be ideal. By means of this, the drying process model will correspond to heating the biomass directly with hot product gas in a stream separated dryer component. Introducing pressure losses in the steam loop, along with realistic isentropic and mechanical efficiencies of the steam blower, will correspond to modelling of the steam drying process of the upscaled two-stage gasification concept. In this study, the steam drying process of the upscaled two-stage gasification concept is used.

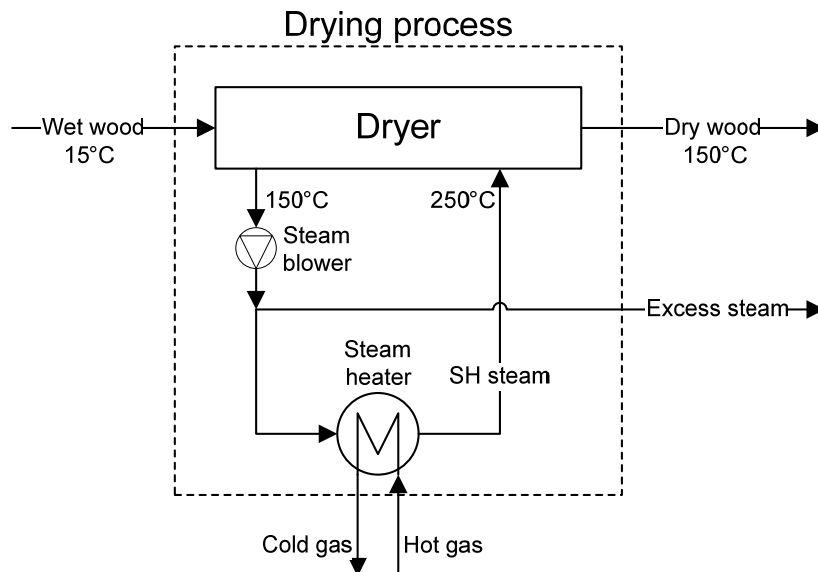


Figure 5.3: Layout of modelled drying process.

The pressure loss in every component in the SOFC air supply stream and burner exhaust stream is assumed to be 10 mbar, whereas the pressure loss in each of the remaining components is assumed to be 5 mbar; the exception being the burner, which has a pressure loss of 0.6‰ of the inlet pressure. In [2], a pressure loss of 4.9 mbar is reported for the gas cleaner in the Viking gasifier, which fits well with the 5 mbar assumption used here. The pressure

losses defined in the peripheral components are shown in Table 5.7 along with other inputs.

Table 5.7: Direct inputs to the peripheral equipment

<i>Heat exchangers</i>			
	$\Delta p_{\text{hot side}} / \text{mbar}$	$\Delta p_{\text{cold side}} / \text{mbar}$	$\Delta T_{\text{pinch}} / ^\circ\text{C}$
Air preheater (gasifier)	5	5	20
Steam heater (dryer)	5	5	
Product gas cooler	5	5	
Condenser	5	5	
Product gas preheater ^a	5	5	150
Air preheater (SOFC) ^a	10	10	200
Exhaust cooler	10	5	90
<i>Turbomachineries</i>			
	Isentropic eff. / %	Mechanical eff. / %	
Fuel and air blower ^b	60	98	
Steam blower (dryer)	60	98	
<i>Others</i>			
	$\Delta p_{\text{biomass and steam}} / \text{mbar}$	$x_{\text{H}_2\text{O, dry wood}} / \%$	$T_{\text{SH steam}} / ^\circ\text{C}$
Drying process	5	5	250
Gas cleaner	Δp 4.9 mbar [2]		
Burner	0.6‰		
Inverter (DC to AC)	Efficiency / % 95		
Electric motor ^b	95		

^a Only used in the SOFC and SOFC-MGT configurations.

^b Only used in the SOFC configuration.

As previously mentioned, the pinch point temperature differences in the SOFC air and product gas preheaters and the exhaust cooler are used as indirect inputs to define outlet temperatures. For the case of the SOFC preheaters, and within the studied SOFC operating temperature range, this means that when changing the SOFC operating temperature, the temperature difference between inlet and outlet is kept constant. The condenser removes some of the water content in the product gas, resulting in a water content of 12.7 vol-%. The resulting S/C ratio is 0.41, which is somewhat low, but it is

justified by the very low tar content in the clean product gas and the high fuel utilization in the SOFC. Hoffman et al. [14] used a S/C ratio of 0.5 and a fuel utilization of 30% when successfully operating SOFCs fed with cleaned product gas from the Viking gasifier. As mentioned in Section 2.2.1, increasing the fuel utilization should make SOFCs able to operate at lower S/C ratios. If necessary, water/steam could be added to the product gas stream before the SOFC, but that is not considered in this work.

Because the air and product gas compressors work as blowers in the SOFC scenario, a lower isentropic efficiency of 60% is used in that scenario. The steam blower used for steam drying is acting as a blower in all scenarios.

The gas cleaner component model simply separates all trace species from the product gas stream and adds a pressure loss to the system. The burner component model assumes perfect combustion and calculates the exhaust gas composition and temperature. The only components having a heat loss are the electrical generator/motor and the DC/AC inverter, where conversion losses are applied for either conversion between electrical and mechanical power or conversion from DC to AC electric power.

Chapter 6 SIMULATIONS OF THE CONCEPTUAL PLANT DESIGNS

By use of the developed models, the simulation tool DNA is used to generate system performance results for the plant configurations investigated. The behaviour of the different plant concepts are studied and discussed by varying critical operating conditions, providing an overview of the optimal conditions and performance of each plant configuration.

Detailed descriptions of the simulated system configurations can be found in Chapter 3. The inputs presented in the previous Chapter 4 and Chapter 5 are also used in these simulations unless otherwise stated.

6.1 PARAMETRIC STUDY OF SYSTEM PERFORMANCES

6.1.1 PRESSURE RATIO

The performance of the different system configurations vary greatly with the operating conditions, and the chosen pressure ratio is of great importance to the resulting system performance. As traditionally, the pressure ratio is defined over the air compressor, and, as seen in Figure 6.1, the different system configurations have different optima with regard to this operating pressure ratio. In Figure 6.2, the corresponding turbine inlet temperatures (TIT), turbine outlet temperatures (TOT), and air compressor outlet temperatures (COT) are shown for the two pressurized systems.

When operating at a constant TIT of 900°C, the MGT configuration shows an optimum at a pressure ratio of 3.7, performing with an electric efficiency of 26.8% (LHV). The recuperator ensures an optimum at a relatively low pressure ratio (see explanation in the end of Chapter 3). Obviously, the pressure in the SOFC case is constantly near atmospheric pressure, because the

gain in SOFC performance at elevated pressure is less than the losses associated with generating the higher pressure. This system performs at an electrical efficiency of 43.1% at a pressure ratio close to 1. The SOFC configuration has a higher efficiency because conversion in the SOFCs is more efficient than in the MGT, but the SOFCs cannot utilize all of the fuel. With a fuel utilization of 85%, a substantial portion of the fuel passes through the anode and is converted to heat in the burner. By combining the SOFC and MGT in the SOFC-MGT configuration, this heat can be used for additional electricity production. At the optimum operating pressure ratio of 2.5, the combined system configuration reaches an electrical efficiency of 55.0%, thereby outperforming the two simpler configurations. The substantial increase in efficiency is mainly the result of better utilization of unconverted fuel and excess heat from the SOFCs, but it is also due to the pressurized operation of the SOFCs.

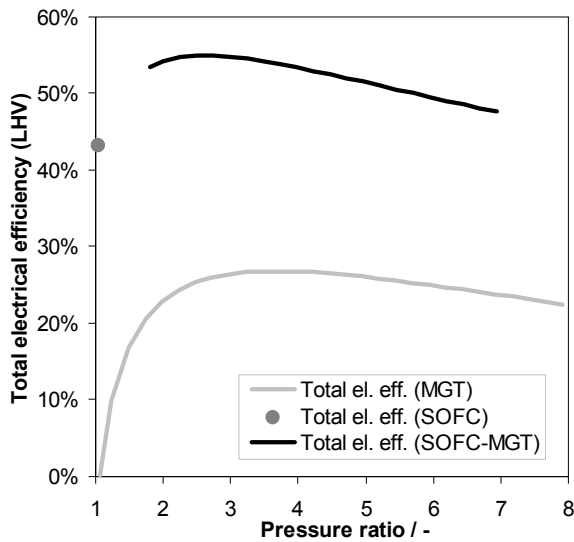


Figure 6.1: Energetic electric efficiency at different operating pressure ratios. The operating pressure ratio is defined over the air compressor.

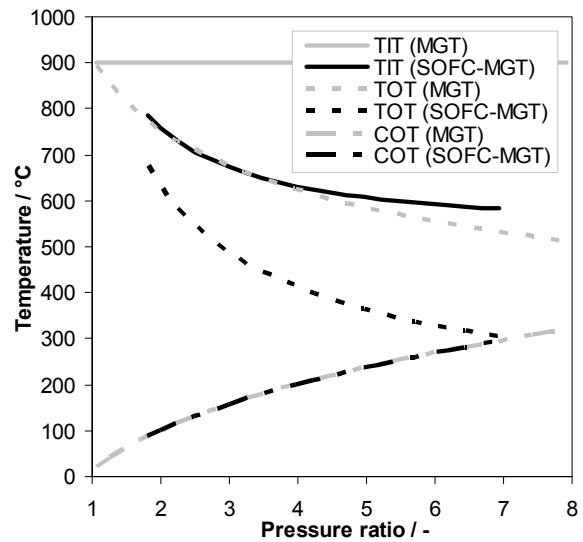


Figure 6.2: Turbine inlet temperatures (TIT), turbine outlet temperatures (TOT), and air compressor outlet temperatures (COT) at different operating pressure ratios. Only the two pressurized system scenarios are illustrated.

In the MGT configuration, the TIT is an input and constant because the air flow fed to the burner is not known from the cooling need of the SOFC stack, contrary to the SOFC-MGT configuration. In the SOFC-MGT arrangement, the TIT decreases with an increasing pressure ratio. This relationship is due to the fact that an increasing PR increases the COT and reduces the TOT, which means that less heat is transferred in the recuperator. Therefore, more heat must be transferred in the SOFC air preheater to reach the same cathode inlet temperature. More heat transfer in the SOFC air preheater results in a lower temperature of the cathode off gas fed to the burner,

thus decreasing the TIT. Furthermore, the TIT is lower in the SOFC-MGT case compared to the MGT scenario because less fuel is used to produce heat in the burner. A TIT of 706°C is reached at a $PR=2.5$. The optimal PR is lower in the SOFC-MGT scenario relative to the MGT arrangement due to the lower TIT. Characteristically, lowering the TIT of a recuperated gas turbine will lower the optimal PR . The slight increase in the SOFC efficiency observed with increasing pressure is not sufficient to change the resulting electrical efficiency trend of the hybrid system. Note that above a PR of approximately 6.7 in the SOFC-MGT case, the TOT becomes lower than the COT, making it impossible to use a recuperator. Below a $PR=1.8$, the heat transfer in the recuperator is sufficiently high to heat the air above the desired cathode inlet temperature.

6.1.2 OPERATING MGT/SOFC TEMPERATURE

The performance of the MGT configuration is also dependent on the allowed TIT as depicted in Figure 6.3. Decreasing the TIT by 100°C to 800°C lowers the electrical efficiency to 24.3% - a drop of 2.5 percentage points. Considering the SOFC configuration, the sensitivity to the SOFC operating temperature is even greater than the sensitivity to the TIT in the MGT case. Lowering the SOFC operating temperature by 100°C to 700°C decreases the electrical efficiency to 32.8% - a drop of 10.3 percentage points. This differential effect indicates that the SOFC operating temperature has a greater influence on SOFC performance than the TIT has on MGT performance in the mentioned temperature range. In the SOFC-MGT configuration, a drop in the SOFC operating temperature of 100°C to 700°C decreases the electrical efficiency to 47.2% - a drop of 7.8 percentage points. Furthermore, the two scenarios incorporating SOFC technology reveals an optimum operating SOFC temperature of approximately 900°C. This is a result of a reducing reversible efficiency of the SOFC with increasing temperature, which also was illustrated in the parametric study of the SOFC model, see Figure 4.13. In the SOFC-MGT scenario, the SOFC operating temperature cannot get below approximately 650°C, because at such a low operating temperature, the recuperator heats the air intake above the desired cathode inlet temperature.

The progress in research and development aimed at lowering the SOFC operating temperature may facilitate the use of cheaper materials, but will also influence the system performance. Figure 6.3 does not give a truthful picture of how much the SOFC performance is affected when lowering the operating temperature through serious research efforts, because it must be expected that a goal of these research efforts is to keep a reasonable SOFC performance even at lower operating temperatures. Therefore, the SOFC component model used in these studies cannot predict the correct SOFC ef-

efficiency of newly or future developed intermediate temperature SOFCs. Undoubtedly though, lowering the operating temperature of the SOFCs in the SOFC-MGT configuration will affect the rest of the electricity producing process causing the system performance to decrease. As mentioned and shown in Figure 6.3, the MGT performance decreases when lowering the TIT, and in the SOFC-MGT configuration, the TIT is also sensitive to the chosen SOFC operating temperature. This is clear from the slope of the TIT as a function of the SOFC operating temperature in the SOFC-MGT configuration illustrated in Figure 6.3. The slope is less steep in the SOFC-MGT configuration than in the MGT case, though, because a lower SOFC operating temperature will cause less preheating of the SOFC inlets to ensure maintenance of the same temperature difference across the electrodes. From this, it is evident that a change in the SOFC operating temperature has reduced impact on the temperature of the anode and cathode off gases fed to the burner, hence also the resulting TIT.

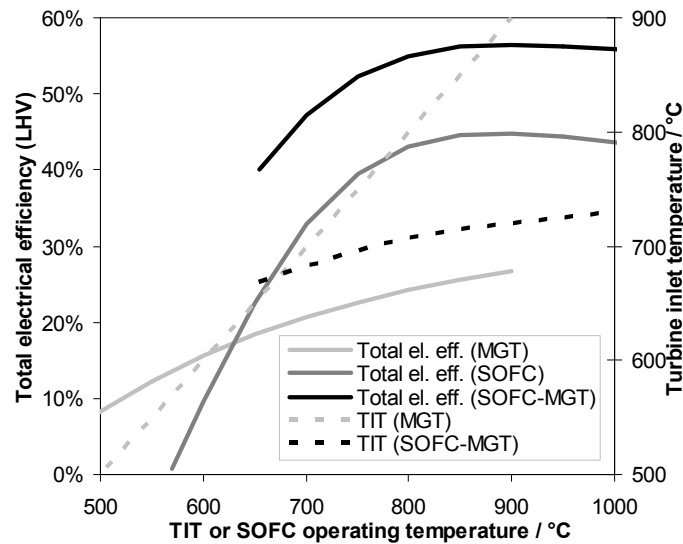


Figure 6.3: Energetic electric efficiency and TIT at different TIT or SOFC operating temperatures. The TIT in the MGT configuration is defined at the gas turbine inlet and the SOFC operating temperature in the two other configurations is defined at the anode/cathode outlets. The maximum allowed TIT is 900°C.

Potentially other bottoming cycles could be beneficial, e.g., a Rankine cycle, if the SOFC operating temperature is lowered. For the scale considered here, a traditional Rankine cycle based on steam would not be feasible, but Rankine cycles based on alternative working fluids could be relevant – i.e., organic Rankine cycles (ORCs). ORC system outputs can range from the kW_e to the MW_e scale, the working fluid can be tailored to let the ORC meet

the required conditions from the topping system, and the process allows the use of low temperature heat sources [73] [74]. It is outside the scope of this work to study possible plant configurations incorporating an ORC, but it should also be mentioned that it seems possible to include both a MGT and an ORC according to Invernizzi et al. [75], hence increasing the performance of the bottoming process producing electricity from the product gas.

Due to the technology development trends, a MGT development that allows for a higher TIT and an SOFC development that enables lowering of the SOFC temperature could lessen the gap between the electrical efficiencies of the MGT and the SOFC configurations. No matter what, the scenario using both SOFCs and a MGT will still be the most efficient plant configuration of the studied.

6.1.3 FUEL UTILIZATION IN SOFCs

The amount of product gas that is utilized in the SOFCs affects the system performances in the SOFC and SOFC-MGT scenarios. The reference value of U_F is 85%. As illustrated in Figure 6.4, the system electrical efficiency decreases with decreasing fuel utilization in the SOFCs. This seems obvious in the SOFC configuration because the excess fuel is only producing heat in the burner. In the SOFC-MGT arrangement, the excess fuel is utilized in the MGT, but the electrical efficiency of the MGT is lower than that of the SOFCs ensuring a decreasing system performance trend with decreasing fuel utilization. The sensitivity to the fuel utilization is slightly greater in the SOFC scenario.

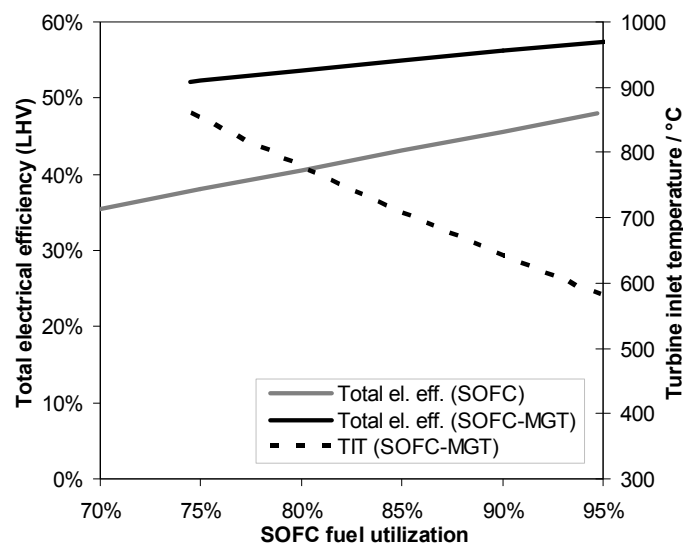


Figure 6.4: Energetic electrical efficiency and TIT as a function of SOFC fuel utilization.

The TIT in the SOFC-MGT configuration turns out to be significantly sensitive to the chosen U_F . The TIT increases from 706°C to 852°C when decreasing the fuel utilization from 85% to 75%. Thereby, the TIT approaches the maximum value of 900°C. Below approximately 75% fuel utilization in the SOFC-MGT scenario, the recuperator heats the air to a temperature above the desired cathode inlet temperature due to the higher TIT, and thereby TOT. This narrows the operational window of possible fuel utilization factors in the SOFC-MGT configuration when using a recuperator, whereas the SOFC scenario can operate at much lower fuel utilization (down to approximately 25% has been successfully simulated). As described in the parametric study of the SOFC performance in Section 4.2, the fuel flow contributes significantly to the SOFC cooling at very low fuel utilization causing a lower air flow (the air flow is controlled by the cooling need to maintain the operating temperature). Thus, the SOFC system configuration also meets a lower fuel utilization limit, when the reduced air flow lowers the SOFC performance significantly. The exact lower fuel utilization limit in the SOFC scenario has not been determined in this study because it is not of interest to operate at very low fuel utilization.

With respect to the system electrical efficiency, it can be concluded that the fuel utilization in the SOFCs should be maintained at a high level. In the SOFC-MGT arrangement, it should also be noted that the fuel utilization factor can be regulated to adjust the TIT to a desired level.

6.1.4 TEMPERATURE GRADIENT OF SOFC CATHODE

An important aspect of SOFC systems is SOFC cooling. Given the SOFC inlet and outlet temperatures are fixed, air flow through the cathode is determined by the cooling requirement of the SOFCs in order to maintain a certain operating temperature. In Figure 6.5, the cathode inlet temperature is varied. It is equivalent to changing the temperature gradient across the cathode (ΔT_c). A higher inlet temperature (a lower ΔT_c) decreases the electrical efficiency of the system. This effect is more pronounced in the SOFC-MGT configuration than in the SOFC case. An increase in the cathode inlet temperature from 600 to 680°C results in a decrease in the electrical efficiency of the SOFC-MGT arrangement from 50.3% to 44.1%, while it only drops from 36.4% to 35.9% in the SOFC configuration. In the SOFC scenario, the air compressor (working as a blower) consumes more power when the ΔT_c is decreased because a higher mass flow of air must be fed to the cathode to ensure a constant SOFC temperature. Thus, the parasitic losses increase, which in turn, slightly lower the electrical efficiency of the system. In the SOFC-MGT arrangement, the higher mass flow of air also passes through the MGT expander, thereby compensating for the greater air compressor work. The higher sensitivity to the chosen cathode inlet temperature in the

SOFC-MGT scenario is explained by the following two facts: One, a lower ΔT_c results in a lower temperature of the cathode off gas fed to the burner (more heat transfer in the SOFC air preheater), and consequently, a lower TIT; and two, a lower ΔT_c necessitates a higher mass flow of air to maintain the same SOFC operating temperature, which ensures a more lean mixture in the burner and thereby decreases the TIT. Therefore, lowering the ΔT_c lowers the TIT, which decreases the MGT output and hence the electrical efficiency of the SOFC-MGT system.

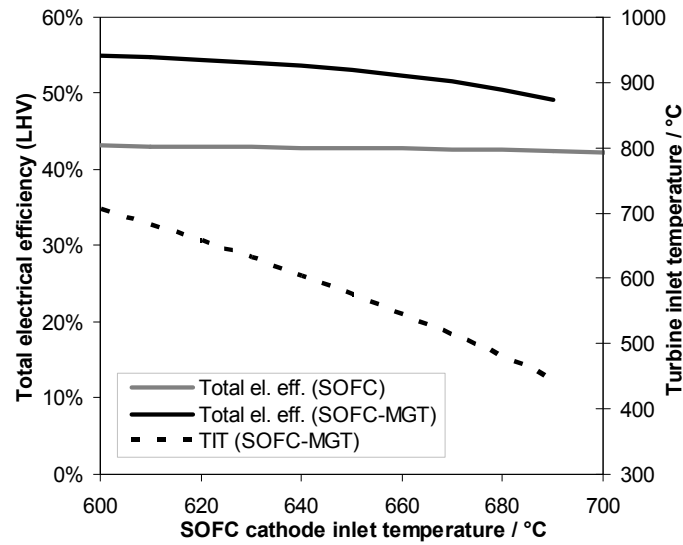


Figure 6.5: Energetic electrical efficiency and TIT as a function of SOFC cathode inlet temperature.

6.1.5 SOFC CURRENT DENSITY

The sensitivity of the model results to the chosen SOFC current density is shown in Figure 6.6. At the reference current density value of 300 mA cm^{-2} , the SOFC efficiency (defined in eq. (4.12)) is 49.5% in the SOFC configuration and 50.7% in the SOFC-MGT arrangement. The difference in SOFC efficiencies is due to the higher SOFC operating pressure in the SOFC-MGT case. Raising the SOFC load to 500 mA cm^{-2} reduces the SOFC efficiencies to 43.9% and 45.1% in the SOFC and SOFC-MGT scenarios, respectively. These decreases result in reductions in the total electrical efficiency to 37.9% and 51.1% - equivalent to respective losses of 5.2 and 3.9 percentage points. These losses cause relative changes in electrical efficiency of 12.1% and 7.1%, respectively, for a 66.7% increase in current density. Therefore, the model is only moderately sensitive to the chosen current density. Furthermore, it is evident that a downstream MGT can raise the electrical efficiency of the total system above the performance of the SOFC alone. As

mentioned earlier, this benefit is due to the utilization of excess fuel from the SOFCs. The sensitivity of the system electrical efficiency to the current density is also slightly reduced when including a MGT.

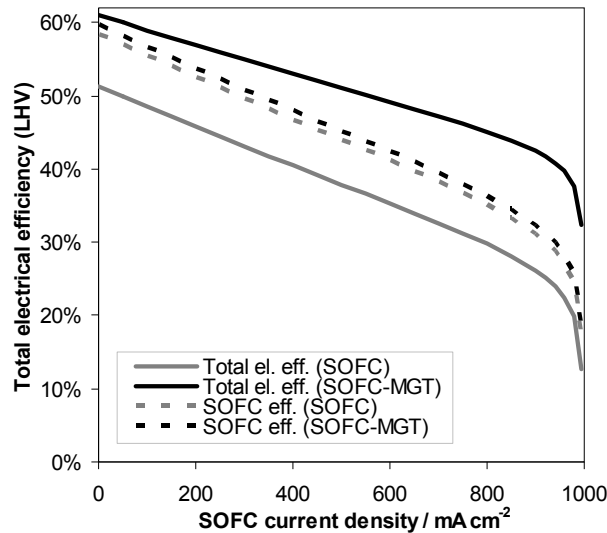


Figure 6.6: System electrical efficiency and SOFC efficiency as a function of SOFC current density.

6.1.6 COLD AND PARTLY DRIED PRODUCT GAS TEMPERATURE (AND S/C)

In the demonstrated Viking gasification plant, the product gas is cooled to 50°C to condense some of the water in the gas before feeding it to a gas engine. This temperature of 50°C after the condenser is also used in this study, but the influence of varying this parameter is examined below.

First of all, the resulting system electrical efficiencies of the three studied scenarios are not affected significantly, as shown in Figure 6.7, when changing the product gas temperature after the condenser from 40°C to 90°C. This temperature cannot reach levels below 40°C because the coolant (DH water) in the inlet to the condenser is 30°C (assuming a pinch temperature difference of 10°C). Since the gas cleaner, situated upstream relative to the condenser, operates at 90°C, the product gas temperature after the condenser can only reach 90°C (without any cooling in the condenser). Surprisingly, the trends in Figure 6.7 seem to change around 55°C. This can be explained by Figure 6.8, where the S/C ratio is illustrated. The S/C ratio is similar in all three concepts. Above approximately 55°C, the condenser only cools the product gas without condensing any water, while below approximately 55°C, water is condensed thereby changing the gas composition. This

change in gas composition explains the change in trends around 55°C. It should be noted, that lowering the S/C ratio increases the risk of carbon deposition. Without any condensing, a S/C ratio of 0.51 is obtained, while at the reference temperature of 50°C, the S/C ratio is 0.41. As mentioned in the end of Section 2.2.1, it seems plausible to operate SOFCs on product gas from the Viking gasifier with a S/C ratio of around or just below 0.5 and still avoid carbon deposition.

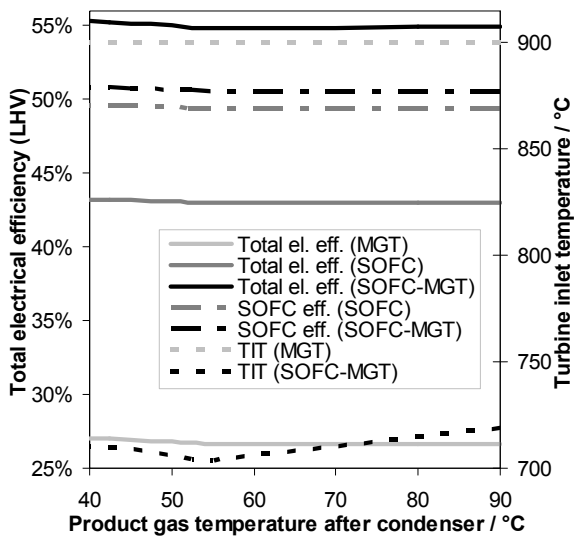


Figure 6.7: Energetic electric efficiency at different product gas temperatures leaving the gasification part of the hybrid system. Note, the scale of the electrical efficiency on the y-axis is narrower than the rest of the figures in this Chapter.

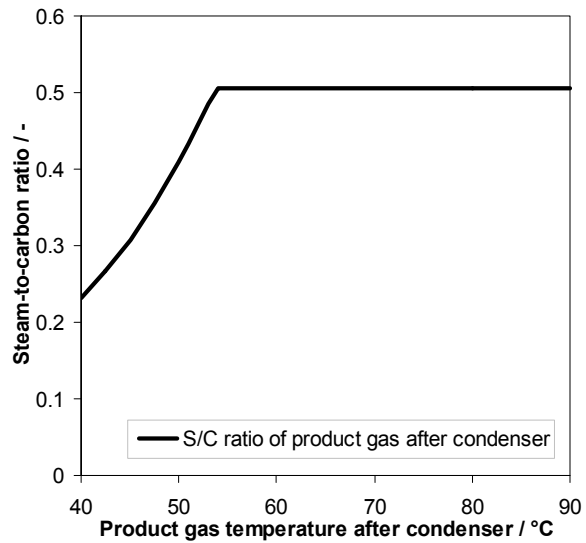


Figure 6.8: Steam-to-carbon ratios at different product gas temperatures leaving the gasification part of the hybrid system.

Decreasing the product gas temperature after the condenser from 55°C improves the efficiency of the MGT system. This is due to two facts: One, the fuel compressor work decreases; and two, a lower S/C ratio ensures a less dilute fuel. The lower fuel compressor work is caused by a lower mass flow and a cooler compressor inlet. The SOFC efficiency is constant at constant S/C ratio, while at decreasing S/C ratio, the SOFC performance increases due to a less dilute fuel. The same trend is seen for the system performance in the SOFC scenario. A lower product gas temperature before the fuel compressor will, as in the MGT case, decrease the power consumption of the compressor, but since it only works as a blower in this scenario, the impact is even less than in the MGT configuration. As for the two other scenarios, the SOFC-MGT case also benefits from a less dilute fuel, when the product gas temperature after the condenser is below 55°C. Besides the increase in SOFC performance, also the MGT performance in the SOFC-MGT arrangement increases when lowering the S/C ratio illustrated by the increas-

ing TIT. Above 55°C the trend is different; an increasing product gas temperature at the fuel compressor inlet increases the TIT. The performance gain from an increased TIT exceeds the performance drop from higher power consumption by the fuel compressor.

All in all, the choice of product gas temperature after the condenser is unimportant to the system performance, but can be relevant because of the varying S/C ratio. The condenser could be removed to reduce plant complexity.

6.1.7 ISENTROPIC EFFICIENCY OF AIR COMPRESSOR/BLOWER

To investigate the influence of the turbomachinery performance, the isentropic efficiency of the air compressor has been varied. A similar study could also be done using the MGT expander or product gas compressor, but that is not performed here. Instead, the air compressor is chosen to represent the turbomachinery. The majority of the required compressor work is consumed by the air compressor because the mass flow of air is significantly larger than the mass flow of product gas.

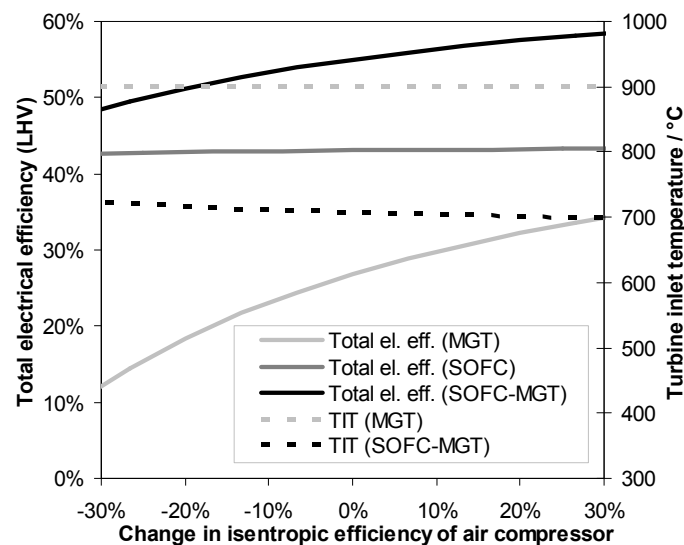


Figure 6.9: System electrical efficiency and TIT as a function of a relative change in the isentropic efficiency of the air compressor.

In Figure 6.9, the system performance is illustrated by the total electrical efficiency and TIT as a function of a relative change in the isentropic efficiency of the air compressor. A relative change is used because the isentropic efficiency of the air compressor in the SOFC configuration is lower than in the two other scenarios (the air compressor works as a blower in the non-pressurized SOFC configuration). The reference values of the isentropic

efficiencies used can be found in Table 5.6 and Table 5.7. The sensitivity of the system performance to the air compressor performance in the SOFC arrangement is insignificant – at least within a range of the relative change in isentropic efficiency of $\pm 30\%$. This is due to the fact that the power consumption from turbomachineries in the SOFC configuration is not significant compared to the net power production of the system. In the two pressurized system arrangements, the sensitivity is greater. It is greatest in the MGT case, where a 20% decrease in the isentropic efficiency results in a system electrical efficiency of 18.4% – a drop of 8.4 percentage points or 31%. In the SOFC-MGT case, a 20% decrease in the isentropic efficiency results in a system electrical efficiency of 51.2% – a drop of 3.8 percentage points or 7%. This clearly shows that the SOFC-MGT arrangement is only moderately sensitive to the air compressor performance, whereas the MGT scenario is highly sensitive. The TIT is constant in the MGT configuration (input), while a slightly decreasing trend of the TIT can be seen at increasing air compressor performance in the SOFC-MGT arrangement. The slight decrease is caused by a reduced amount of heat generation in the air compressor at increasing compressor performance. The TIT is not affected significantly, though.

6.1.8 SUMMARY

The parametric study of the system performances has revealed different trends and optima as well as windows of possible operation. Here follows a summary of the findings.

The MGT scenario showed a high sensitivity to the chosen pressure ratio and revealed an optimum of 3.7. The choice of turbine inlet temperature also turned out to greatly influence the MGT performance, and it can be concluded that the TIT should be maximized (limited by material constraints). Infinitesimal influence on the MGT system performance was shown from the chosen product gas temperature after the condenser in the gasifier plant part, and the resulting S/C ratio does not seem important to the MGT configuration. The condenser could be removed to reduce cost and plant complexity. Finally, the chosen isentropic efficiency of the air compressor affected the MGT system significantly.

The SOFC system configuration was not pressurized, so the operating pressure ratio was constantly around 1. The choice of operating temperature of the SOFC had great influence on the SOFC system performance and actually revealed an optimum at approximately 900°C, which is higher than the reference value of 800°C. From a system electrical efficiency point of view, the SOFC operating temperature should be maintained at a high level. The fuel utilization factor should also be maintained at a high level because the

excess fuel is not used to produce additional power in this scenario. Within the studied range of temperature differences across the cathode, significant impact on the system performance was not shown. From an efficiency point of view, the SOFC current density should be minimized, but a lower current density will also result in a lower power production. Since the investment cost of SOFCs is significant in this kind of system, it will not be feasible to minimize the current density, but rather to determine the optimal current density from an economical viewpoint. As for the MGT scenario, the chosen product gas temperature after the condenser has infinitesimal influence on the SOFC system performance. Contrary to the MGT case, the resulting S/C ratio can be important to avoid carbon deposition in the SOFCs. If a higher S/C ratio is needed, the product gas temperature after the condenser could be increased or the condenser removed. Since the SOFC arrangement is not pressurized, the sensitivity of the system performance is not affected significantly by the performance of the turbomachineries.

In the SOFC-MGT scenario, similar to the MGT case, the pressure ratio affected the system performance significantly and an optimum was found at a pressure ratio of 2.5. The influence on the system electrical efficiency of varying the SOFC operating temperature revealed an optimum around 900°C. Like in the SOFC configuration, it is recommended to maintain a high SOFC operating temperature in the SOFC-MGT scenario. When combining SOFCs and a MGT, the SOFC fuel utilization factor should still be maintained at a high level from a system electrical efficiency viewpoint, but the parametric study also revealed that the fuel utilization in the SOFCs can be varied to regulate the turbine inlet temperature. Contrary to the SOFC configuration, the temperature difference across the cathode showed a moderate influence on the system performance. In this case, the temperature difference should be maximized (limited by thermal stresses in the SOFCs) to keep a high turbine inlet temperature. As mentioned in the SOFC case above, the current density should be minimized from an efficiency viewpoint, but optimized from an economical viewpoint. In any case, the current density has significant impact on the system performance. The choice of product gas temperature after the condenser was unimportant to the system electrical efficiency, but, as for the SOFC case, the resulting water content or S/C ratio can influence the risk of carbon deposition in the SOFC. Finally, the system performance showed significant sensitivity to the isentropic efficiency of the air compressor.

Generally, it can be concluded, that inclusion of a MGT in an SOFC system, besides increasing the system electrical efficiency, ensures a lower sensitivity of the electrical efficiency to operating conditions of the SOFCs. If the SOFC performance for some reason decreases it will produce less electricity but additional heat. The additional heat can be utilized by the MGT, though

at a lower conversion efficiency. Even more generally, it can be stated that combining SOFCs with downstream heat engines ensures a system performance with a higher robustness to conditions causing varying SOFC performance. On the other hand, the operational window of the SOFC-MGT configuration is limited compared to the MGT scenario and SOFC scenario.

6.2 KEY DATA

Key data from the three studied plant configurations are presented in Table 6.1. The gasifier plant part is similar in all configurations, performing with a cold gas efficiency of 94.0% and an exergy efficiency of 80.8%. The subsystems converting the product gas to power and heat are where the studied systems differ. The respective optimal pressure ratio in each configuration is used besides the reference input values presented in Chapter 4 and Chapter 5. The SOFC-MGT subsystem clearly has the best energetic and exergetic electrical efficiencies. Notably, the exergy electrical efficiencies of the subsystems are slightly higher than the corresponding energy-based ones. This is because the exergy content in the input product gas fed to the subsystem is lower than the energy content. In the demonstrated Viking gasifier, the product gas is converted to electric power by an internal combustion gas engine and a generator at an efficiency of 29.1% [11]. Thus, the MGT does not seem better than a gas engine – especially when considering that the gas engine would be expected to achieve a higher efficiency at the scale of the studied plant configurations. As expected, the SOFC stack appears to be the most efficient power producing single technology of the considered. In the SOFC-MGT case, power production is mainly derived from the SOFCs, which produce 82-83% of the net AC power, when accounting for the power consumption of the compressors in the MGT net power production. In the SOFC configuration, the power consumption from the compressors is accounted for in the SOFC net power production, but the power consumption is much lower because of no pressurization.

Considering the total systems, the electrical efficiencies are slightly lower because the losses of the gasifier plant are included. The CHP efficiencies, or cogeneration efficiencies, do not differ significantly in the two scenarios including SOFCs, but in the MGT case, the CHP efficiency is lower. This is governed by the heat loss through the flue gas exiting the plant, which is greatest in the MGT configuration because of a higher air and exhaust flow. The higher air flow also explains the higher exergetic input through the air fed to the subsystem in the MGT arrangement.

Table 6.1: Key data for the studied plant configurations.

	Gasifier- MGT	Gasifier- SOFC	Gasifier- SOFC-MGT
<i>Gasifier plant key data</i>			
Biomass throughput / kg h^{-1}	154.8	154.8	154.8
Energetic biomass input ($\dot{m}_{\text{biomass}} LHV_{\text{biomass}}$) / kW_{th}	499.2	499.2	499.2
Exergetic biomass input ($\dot{\Psi}_{\text{biomass}}$) / kW	572.4	572.4	572.4
Exergetic air input to gasifier ($\dot{\Psi}_{\text{air,gasifier}}$) / kW	0.2	0.2	0.2
Steam blower power ($P_{\text{steam blower}}$) / kW	0.7	0.7	0.7
Energetic product gas output ($\dot{m}_{\text{PG}} LHV_{\text{PG}}$) / kW_{th}	469.1	469.1	469.1
Exergetic product gas output ($\dot{\Psi}_{\text{PG}}$) / kW	463.1	463.1	463.1
$\eta_{\text{cold gas}}$ / % ^a	94.0	94.0	94.0
$\eta_{\Psi,\text{gasifier plant}}$ / % ^b	80.8	80.8	80.8
<i>Subsystem key data</i>			
PR / -	3.7	1.04	2.5
Exergetic air input to subsystem ($\dot{\Psi}_{\text{air,subsystem}}$) / kW	4.9	3.6	3.5
MGT net power production ($P_{\text{net,MGT}}$) / kW_e	134.5 ^c	-	48.5 ^c
SOFC net power production ($P_{\text{net,SOFC}}$) / kW_e	-	215.7 ^c	226.7
SOFC cell potential (V_{cell}) / V	-	0.800	0.820
$\eta_{\text{el,subsystem}}$ / % ^d	28.7	46.0	58.7
$\eta_{\Psi,\text{el,subsystem}}$ / % ^e	28.7	46.2	59.0
<i>Total system key data</i>			
Total net power production ($P_{\text{net,tot}}$) / kW_e ^f	133.8	215.0	274.5
Total district heating production (Q_{DH}) / kJ s^{-1}	240.3	199.0	137.8
Exergy of heat production ($\dot{\Psi}_{\text{DH}}$) / kW	29.0	24.0	16.6
$\eta_{\text{el,total system}}$ / % (LHV) ^g	26.8	43.1	55.0
$\eta_{\text{CHP,total system}}$ / % (LHV) ^h	74.9	82.9	82.6
$\eta_{\Psi,\text{el,total system}}$ / % ⁱ	23.2	37.3	47.6
$\eta_{\Psi,\text{CHP,total system}}$ / % ^j	28.2	41.5	50.5

^a Defined in eq. (2.8).

^b Defined as $\eta_{\Psi,\text{gasifier plant}} = \dot{\Psi}_{\text{PG}} / (\dot{\Psi}_{\text{biomass}} + \dot{\Psi}_{\text{air,gasifier}} + P_{\text{steam blower}})$.

^c Power consumption of the fuel and air compressors/blowers are included here.

^d Defined as $\eta_{\text{el,subsystem}} = (P_{\text{net,MGT}} + P_{\text{net,SOFC}}) / (\dot{m}_{\text{PG}} LHV_{\text{PG}})$.

^e Defined as $\eta_{\Psi,\text{el,subsystem}} = (P_{\text{net,MGT}} + P_{\text{net,SOFC}}) / (\dot{\Psi}_{\text{PG}} + \dot{\Psi}_{\text{air,subsystem}})$.

^f Including steam blower power consumption.

^g Defined as $\eta_{\text{el,total system}} = P_{\text{net,tot}} / (\dot{m}_{\text{biomass}} LHV_{\text{biomass}})$.

^h Defined as $\eta_{\text{CHP,total system}} = (P_{\text{net,tot}} + Q_{\text{DH}}) / (\dot{m}_{\text{biomass}} LHV_{\text{biomass}})$.

ⁱ Defined as $\eta_{\Psi,\text{el,total system}} = P_{\text{net,tot}} / (\dot{\Psi}_{\text{biomass}} + \dot{\Psi}_{\text{air,gasifier}} + \dot{\Psi}_{\text{air,subsystem}})$.

^j Defined as $\eta_{\Psi,\text{CHP,total system}} = (P_{\text{net,tot}} + \dot{\Psi}_{\text{DH}}) / (\dot{\Psi}_{\text{biomass}} + \dot{\Psi}_{\text{air,gasifier}} + \dot{\Psi}_{\text{air,subsystem}})$.

tem part were 46.4%, 48.9%, and 50.8% for air, oxygen, and steam, respectively (LHV). In this study, the efficiency reaches 58.7% (LHV). The gasifying agent in the two-stage gasification concept is a mixture because air is used for partial oxidation but steam and CO_2 are used for gasifying the char. The lower efficiency in the study by Sucipta et al. is due to a lower electrical efficiency of the SOFCs, between 35% and 38% (LHV), whereas the SOFCs in this study reach approximately 50%. A fuel utilization of 85% is used in both studies, while the current density, temperature, and pressure ratio are 300 mA cm^{-2} , 800°C , and 2.5 in this study and were 320 mA cm^{-2} , $900\text{-}950^\circ\text{C}$, and 2.9 in the study by Sucipta et al. Sucipta et al. used a S/C ratio of 2.5 (0.41 in this study), which could be part of the reason. The SOFCs modelled by Sucipta et al. are tubular, but it is not clear whether the model is calibrated against experimental data or not.

The total plant performance of the SOFC-MGT scenario can be compared to the results of Fryda et al. [44] and Barchewitz and Palsson [38]. As described in Section 2.4, an autothermal (air) biomass gasifier feeding an SOFC and recuperated MGT system performed with a net electrical efficiency of the complete plant of 40.6% (LHV) in the study by Fryda et al. The reason for the lower efficiency in the study by Fryda et al. compared to this study is partly a lower cold gas efficiency of the gasifier, substantial heat losses in the gas cleaning system, a higher S/C ratio of 2, and a lower SOFC performance. The modelled SOFC in the work by Fryda et al. was operated at 85% fuel utilization, a current density of 428 mA cm^{-2} , a temperature of 900°C , and a pressure of 4 bar. The operating pressure was not optimized with respect to the net electrical efficiency of the hybrid system, though. In the study by Barchewitz and Palsson, a pressurized autothermal air-blown circulating fluidized bed gasifier fed planar SOFCs with a bottoming recuperated gas turbine. This plant reached a net electrical efficiency of 58.5% (LHV) at an optimal pressure of 2.65 bar, which is higher than the performance of 55.0% (LHV) found in this study. The size of the plant in the study by Barchewitz and Palsson was 4-5 MW_e , so better turbomachinery and a higher TIT were used compared to this study, which explains the better performance.

From two of the three comparisons above, it seems that the modelled SOFC performance in this study is relatively high. This impression could be caused by too low SOFC performance estimations in the works by Sucipta et al. and Fryda et al., but could also originate from the calibration of the SOFC model in this study. More detailed analysis on the reliability of the SOFC model calibration is left for future work. On the other hand, both the SOFC-MGT plant performance and optimal pressure ratio fit well with the results from the work by Barchewitz and Palsson.

Chapter 7 OPTIMIZATION OF THE SOFC-MGT SCENARIO

Based on the findings in the previous Chapter, the SOFC-MGT scenario has been chosen for optimization. The optimization is based on 1st and 2nd law analyses. The plant model listing for the optimized SOFC-MGT scenario can be found in Appendix F.

7.1 1ST AND 2ND LAW ANALYSES

1st law efficiency is defined as the ratio of useful energy products to total energy inputs, and by use of 1st law analysis the plant performance can be evaluated as seen in the presented results (cf., Table 6.1). 2nd law efficiency is defined congruently as the ratio of exergy in useful products (e.g., electrical power) to total exergy inputs, and by use of 2nd law analysis (often called exergy analysis) inefficiencies due to irreversibilities within the plant can be located.

A Sankey diagram of the energy flows in the SOFC-MGT configuration is presented in Figure 7.1. The Sankey diagram clearly shows the flow of energy, e.g., it clearly shows that a substantial heat amount is transferred from the anode to the cathode. The energy transferred through the membrane is calculated by 1st law balancing of one of the electrodes, but the O²⁻ flow from the cathode to the anode is not differentiated from the heat flow from the anode to the cathode. Therefore, the illustrated energy flow is a net energy flow between the electrodes. Besides that, it is apparent how important the recuperator is as it recovers significant heat amounts for additional power production that else would have been only contributing to a higher district heating production. In addition, it is evident that 55% of the biomass feedstock is converted into net electric power, while about 28% of it is used for producing hot water for district heating purposes. Of the 17% of wasted



1. *Journal of the American Medical Association*, 1997; 277: 1039-1043.

value of heat, especially low-temperature heat, and the high exergetic value of chemical, mechanical, and electrical energy. In Figure 7.2, all the exergy destruction in the SOFCs is applied to the membranes.

The exergy destructions in the different components in Figure 7.2 are illustrated in Figure 7.3. Figure 7.3 clearly shows that the largest exergy destruction lies in the gasification reactor, $77.6 \text{ kW}_{\text{ex}}$, 13% of the plant exergy input and almost 27% of the total exergy loss in the plant. This covers pyrolysis, partial oxidation, and char gasification, though, because these are not separated in the modelling of the gasification process. Furthermore, mixing of steam and air fed to the gasifier accounts for approximately $4.9 \text{ kW}_{\text{ex}}$ of the total $77.6 \text{ kW}_{\text{ex}}$ of exergy destruction in the gasifier. Additionally, $31.2 \text{ kW}_{\text{ex}}$ is leaving the plant in the flue gas and $28.7 \text{ kW}_{\text{ex}}$ is destroyed in the burner. Thus, a bit more than 5% of the plant exergy input and 11% of the total plant exergy loss leaves the plant in the flue gas, while 5% of the exergy input and 10% of the total exergy loss is destroyed in the burner. The exergy destruction in the SOFCs is moderate compared to the other components, $12.9 \text{ kW}_{\text{ex}}$, slightly more than 2% of the plant exergy input and almost 5% of the total exergy loss in the plant.

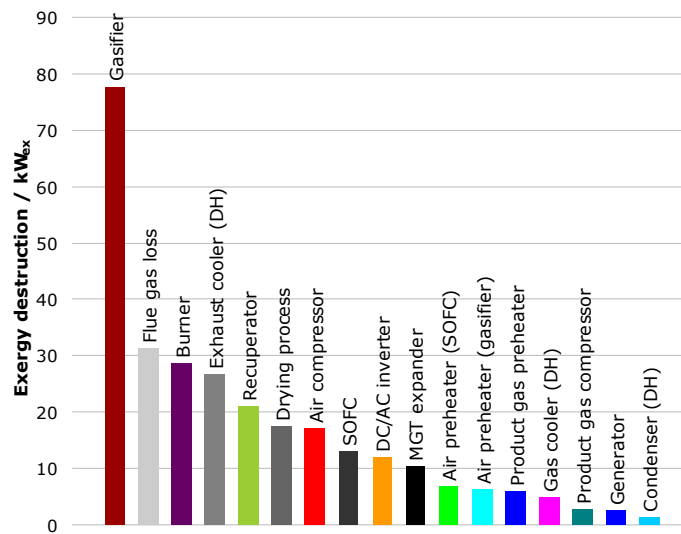


Figure 7.3: Exergy losses and destructions in the different components of the SOFC-MGT plant configuration. Total exergy destruction and loss in the plant is approximately $286 \text{ kW}_{\text{ex}}$.

The exergy destruction in the burner can be divided into contributions from mixing and the irreversible combustion process. Similar issues have been discussed by Dunbar and Lior [77]. Evaluating the exergy destruction in the burner reveals that mixing of the reactants accounts for $15.7 \text{ kW}_{\text{ex}}$, while the

irreversible combustion process accounts for 13.0 kW_{ex}. Of the 15.7 kW_{ex} loss due to mixing, approximately 1.9 kW_{ex} is caused by thermal equilibration, i.e., reaching an even temperature of the mixture. The rest of the mixing loss, 13.8 kW_{ex}, is caused by diffusion. If the anode and cathode off gases fed to the burner had the same temperature, the losses due to thermal equilibration would disappear. In the studied SOFC-MGT scenario, the depleted product gas and air flow fed to the burner have temperatures of 410°C and 684°C, respectively (cf., Figure 6.10).³

Of the total exergy loss of approximately 286 kW_{ex}, almost 28% is lost in heat exchangers and 11% in turbomachineries, underlining the importance of heat exchanger performance. Assuming the gasifier, the SOFCs, the inverter, and the generator are state-of-the-art, minimization of exergy destructions or losses to increase plant performance should be found within the flue gas loss, the burner, the heat exchanger network, and the turbomachinery.

In Table 7.1, the exergy efficiencies of the plant components are listed along with defined inputs and products. The lowest exergy efficiencies are found in the exhaust cooler and product gas cooler, both producing district heating. The reason for the low exergy efficiencies are the great temperature difference between the hot and cold side of the heat exchangers. This indicates a potential for improving the heat exchanger network. Especially the exhaust cooler performance is important because the exergy flow through this component is high and thereby the exergy destruction is significant.

The exergy efficiency of the burner is high, 93.1%, but the exergy destruction is still significant according to Figure 7.3. As for the exhaust cooler, the exergy flow through the burner is high, causing significant exergy destruction despite the high exergy efficiency. As discussed below Figure 7.3, the exergy destruction in the burner could be reduced by having more equal temperatures of the anode and cathode off gases fed to the burner, e.g., by preheating.

The exergy efficiency of the SOFC component is very high, 98.3%, because the high-temperature off gases are considered valued products along with the produced electricity. Obviously, the exergy content of the product gas flow decreases through the SOFCs due to the conversion to electricity, but the exergy content of the air flow increases. The physical exergy content of the SOFC off gases is high due to the high temperature ensuring very high

³ The exergy destruction caused by mixing is determined by evaluating the exergy destruction in a modelled mixer with the same inlet conditions as the burner. The part due to thermal equilibration can be determined by evaluating the reduction in exergy loss when the inlet temperatures are evened out. The rest of the mixing loss is attributable to diffusion.

exergy efficiency. On the other hand, if only the electricity is considered a valued product, the exergy efficiency drops dramatically to only 30.9%. Considering only the chemical exergy of the product gas input and the electricity output, the resulting exergy efficiency of the SOFCs is 51.5%.

Table 7.1: Exergy efficiencies of components from defined inputs and products^a. The components are listed in order according to the exergy destructions seen in Figure 7.3.

Component	Input(s)	Product(s)	$\eta_{\Psi} / \%$
Gasifier	Dry wood, steam, air	Product gas	87.0
Burner	Anode off gas, cathode off gas	Combustion products	93.1
Exhaust cooler (DH)	Exergy decrease of exhaust gas	Exergy increase of DH water	32.6
Recuperator	Exergy decrease of MGT expander exhaust	Exergy increase of air	86.2
Drying process ^b	Wet biomass, heat from product gas, steam blower power	Dry biomass, steam	97.1
Air compressor	Mechanical work	Exergy increase of air	79.8
SOFC	Product gas input, air input	DC electric power, product gas output, air output	98.3
DC/AC inverter	DC electric power	AC electric power	95.0
MGT expander	Exergy decrease of combustion products	Mechanical work	93.6
Air preheater (SOFC)	Exergy decrease of cathode off gas	Exergy increase of SOFC air	89.6
Air preheater (gasifier)	Exergy decrease of product gas	Exergy increase of gasifier air	74.5
Product gas preheater	Exergy decrease of anode off gas	Exergy increase of product gas	84.4
Gas cooler (DH)	Exergy decrease of product gas	Exergy increase of DH water	34.4
Product gas compressor	Mechanical work	Exergy increase of product gas	81.7
Generator	Mechanical work	AC electric power	95.0
Condenser (DH)	Exergy decrease of product gas	Exergy increase of DH water	90.1

^a Defined as $\eta_{\Psi} = \dot{\Psi}_{\text{product}} / \dot{\Psi}_{\text{input}}$.

^b Includes dryer, steam blower, and steam heater (see Figure 5.3).

7.1.1 RECOMMENDATIONS FOR OPTIMIZATION

From the 1st and 2nd law analyses, potential modifications for optimizing the plant performance can be derived. The goals of the optimization are to reduce the exergy losses or destructions of; (1) heat exchanging, (2) the burner, (3) the turbomachinery, and (4) the flue gas leaving the plant. The plant components are assumed to be state-of-the-art, so focus is kept on improving the system layout and operating conditions, e.g., by improving the heat exchanger performances by matching temperature levels, improving the burner performance by increasing the temperatures of the burner inlets, and improving the MGT expander by increasing the TIT. Below, suggested modifications to the SOFC-MGT system are listed.

I. Better Use of Hot Product Gas for Additional Anode Feed Preheating

The product gas leaving the gasifier air preheater has a high temperature of 552°C. In the SOFC-MGT scenario presented above, the hot product gas is used to heat dryer steam from 152°C to 250°C in the steam heater of the drying process. The large temperature difference of the product gas and dryer steam is not favourable, so it is suggested to use the high quality heat of the product gas for something else. Specifically, it is suggested to preheat the pressurized product gas in two steps instead of one, the first being heated by the product gas leaving the gasifier air preheater and the second by the anode off gas. The first preheater should preheat the pressurized product gas as much as possible. Thus, less heat exchange will be necessary in the second step preheater to reach the desired product gas temperature of 650°C at the anode inlet, thereby increasing the temperature of the anode off gas leaving the second preheater and entering the burner. Therefore, introducing a first step product gas preheater will address three of the four established goals. The hot product gas leaving the gasifier air preheater is better utilized, the exergy destruction in the burner is reduced because of the increased temperature of the depleted product gas fed to the burner, and the performance of the MGT expander is improved because of an increased TIT.

II. Use of Exhaust Gas Heat for the Biomass Drying Process

It is suggested to heat the drying process by the flue gas leaving the recuperator. The temperature of the flue gas downstream the recuperator is 245°C in the SOFC-MGT scenario presented above, so, at first, it seems that the superheated steam temperature can only reach up to around 235°C and not the 250°C that is intended. If suggestion I above is implemented, a higher TIT is obtained, thus the TOT and flue gas outlet temperature of the recuperator will also be higher. Therefore, reaching a superheated steam temperature of 250°C is expected to be feasible.

III. Reduce the Stack Temperature

The loss through the flue gas is substantial seen from the 1st law analysis and, surprisingly, also from the 2nd. It is suggested to reduce the stack temperature from 120°C to 90°C to make better use of the excess heat in the exhaust cooler. A stack temperature of 90°C is found to be realistic.

7.2 OPTIMIZED SOFC-MGT SCENARIO

Applying the modifications suggested by the 1st and 2nd law analyses in the previous Section, an optimized SOFC-MGT configuration is simulated. The system layout is presented in Figure 7.4.

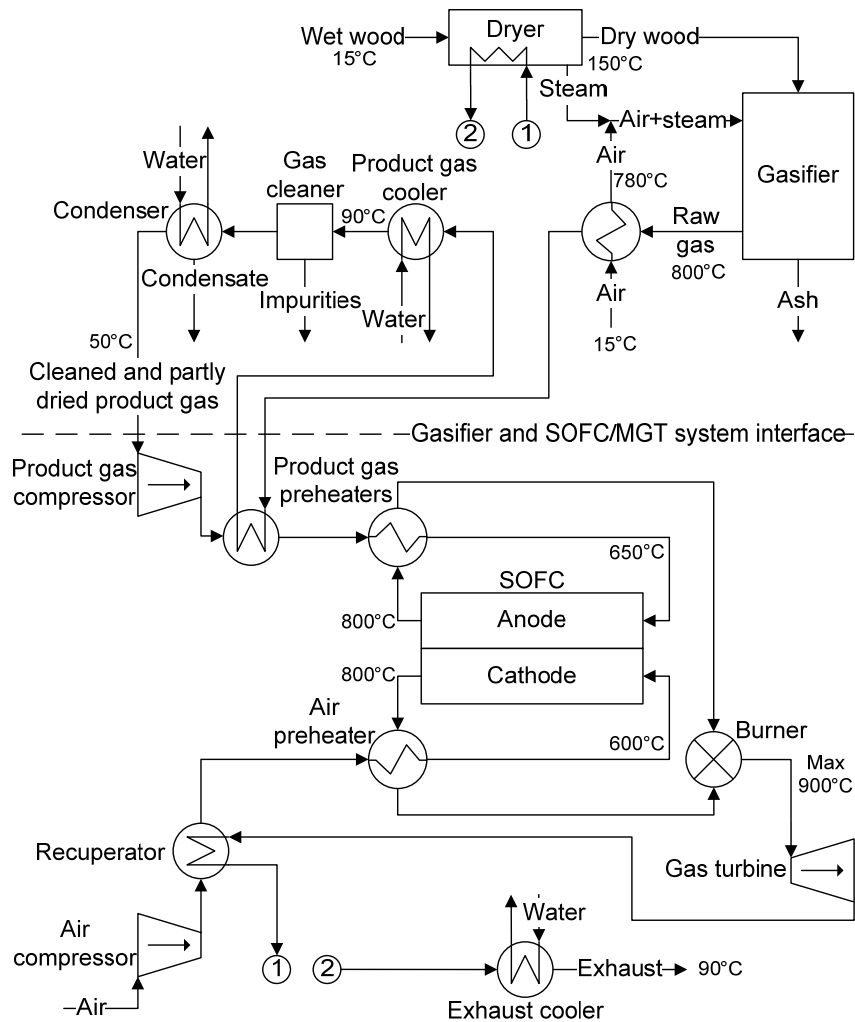


Figure 7.4: System layout of optimized SOFC-MGT scenario.

The exhaust gas downstream the recuperator is delivering heat to the biomass drying process by heating dryer steam in the steam heater (see Figure 5.3). The conditions for the steam heater are the same as in the original SOFC-MGT arrangement (see Table 5.7). The hot product gas leaving the gasifier air preheater, that previously heated the drying process, preheats the pressurized product gas in a first step preheater, while the anode off gas preheats the pressurized product gas in a second step preheater. The added first step preheater ensures a higher temperature of the anode off gas leaving the second step preheater and entering the burner. Since the first step product gas preheater works as a recuperator, a heat exchanger effectiveness of 85% is applied. Pressure drops of 5 mbar are applied to both sides of the first step preheater. Finally, the temperature of the exhaust gas leaving the hybrid system is lowered from 120°C to 90°C.

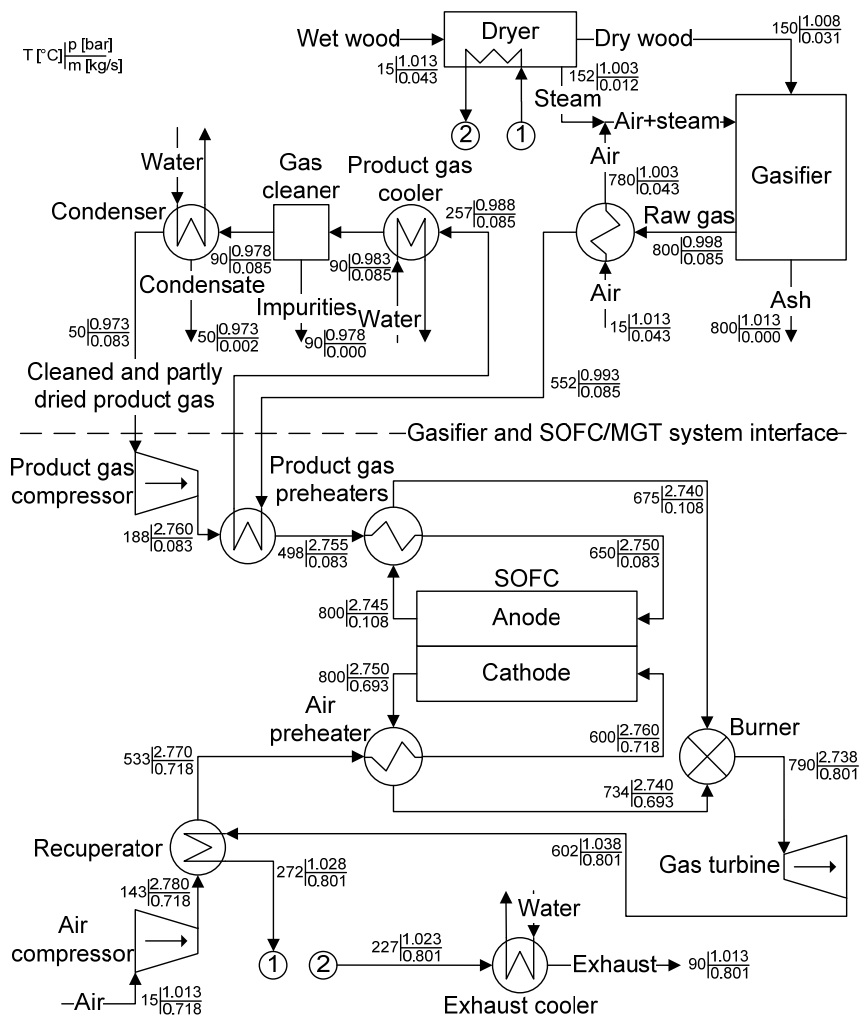


Figure 7.5: Flow sheet of optimized SOFC-MGT configuration with applied temperatures, pressures, and mass flow rates.

Table 7.2: Key data for the original and optimized SOFC-MGT configurations.

	Gasifier-SOFC-MGT	Optimized gasifier-SOFC-MGT
<i>Gasifier plant key data</i>		
Biomass throughput / kg h^{-1}	154.8	154.8
Energetic biomass input ($\dot{m}_{\text{biomass}} LHV_{\text{biomass}}$) / kW_{th}	499.2	499.2
Exergetic biomass input ($\dot{\Psi}_{\text{biomass}}$) / kW	572.4	572.4
Exergetic air input to gasifier ($\dot{\Psi}_{\text{air,gasifier}}$) / kW	0.2	0.2
Steam blower power ($P_{\text{steam blower}}$) / kW	0.7	0.7
Energetic product gas output ($\dot{m}_{\text{PG}} LHV_{\text{PG}}$) / kW_{th}	469.1	469.1
Exergetic product gas output ($\dot{\Psi}_{\text{PG}}$) / kW	463.1	463.1
$\eta_{\text{cold gas}}$ / % ^a	94.0	94.0
$\eta_{\Psi,\text{gasifier plant}}$ / % ^b	80.8	80.8
<i>Subsystem key data</i>		
PR / -	2.5	2.7
Exergetic air input to subsystem ($\dot{\Psi}_{\text{air,subsystem}}$) / kW	3.5	3.5
MGT net power production ($P_{\text{net,MGT}}$) / kW_e ^c	48.5	63.8
SOFC net power production ($P_{\text{net,SOFC}}$) / kW_e	226.7	227.3
SOFC cell potential (V_{cell}) / V	0.820	0.822
$\eta_{\text{el,subsystem}}$ / % ^d	58.7	62.1
$\eta_{\Psi,\text{el,subsystem}}$ / % ^e	59.0	62.4
<i>Total system key data</i>		
Total net power production ($P_{\text{net,tot}}$) / kW_e ^f	274.5	290.4
Total district heating production (Q_{DH}) / kJ s^{-1}	137.8	146.2
Exergy of heat production ($\dot{\Psi}_{\text{DH}}$) / kW	16.6	17.6
$\eta_{\text{el,total system}}$ / % (LHV) ^g	55.0	58.2
$\eta_{\text{CHP,total system}}$ / % (LHV) ^h	82.6	87.5
$\eta_{\Psi,\text{el,total system}}$ / % ⁱ	47.6	50.4
$\eta_{\Psi,\text{CHP,total system}}$ / % ^j	50.5	53.4

^a Defined in eq. (2.8).

^b Defined as $\eta_{\Psi,\text{gasifier plant}} = \dot{\Psi}_{\text{PG}} / (\dot{\Psi}_{\text{biomass}} + \dot{\Psi}_{\text{air,gasifier}} + P_{\text{steam blower}})$.

^c Power consumption of the fuel and air compressors are included here.

^d Defined as $\eta_{\text{el,subsystem}} = (P_{\text{net,MGT}} + P_{\text{net,SOFC}}) / (\dot{m}_{\text{PG}} LHV_{\text{PG}})$.

^e Defined as $\eta_{\Psi,\text{el,subsystem}} = (P_{\text{net,MGT}} + P_{\text{net,SOFC}}) / (\dot{\Psi}_{\text{PG}} + \dot{\Psi}_{\text{air,subsystem}})$.

^f Including steam blower power consumption.

^g Defined as $\eta_{\text{el,total system}} = P_{\text{net,tot}} / (\dot{m}_{\text{biomass}} LHV_{\text{biomass}})$.

^h Defined as $\eta_{\text{CHP,total system}} = (P_{\text{net,tot}} + Q_{\text{DH}}) / (\dot{m}_{\text{biomass}} LHV_{\text{biomass}})$.

ⁱ Defined as $\eta_{\Psi,\text{el,total system}} = P_{\text{net,tot}} / (\dot{\Psi}_{\text{biomass}} + \dot{\Psi}_{\text{air,gasifier}} + \dot{\Psi}_{\text{air,subsystem}})$.

^j Defined as $\eta_{\Psi,\text{CHP,total system}} = (P_{\text{net,tot}} + \dot{\Psi}_{\text{DH}}) / (\dot{\Psi}_{\text{biomass}} + \dot{\Psi}_{\text{air,gasifier}} + \dot{\Psi}_{\text{air,subsystem}})$.

The conditions throughout the system change in the optimized scenario. The resulting temperatures, pressures, and mass flow rates in the different flows can be found in Figure 7.5. Key data for the optimized SOFC-MGT scenario are presented in Table 7.2 along with key data for the original SOFC-MGT scenario.

The system performance clearly improves in the optimized SOFC-MGT arrangement. The net electrical efficiency increases from 55.0% to 58.2% and the exergetic electrical efficiency from 47.6% to 50.4%. It is seen from Table 7.2 that it is mainly an increased net MGT power production that ensures the performance gain. This is due to the increased burner inlet temperatures and TIT. The higher temperature of the air inlet to the burner is caused by a higher TOT and hence a greater air temperature rise in the recuperator. The share of AC power generation from the SOFCs is reduced from 82-83% to approximately 78%. Furthermore, the optimal PR increases from 2.5 to 2.7. As described in Section 6.1.1, a higher TIT moves the optimal PR to a higher level. The slightly increased PR also explains the small increase in SOFC net power output. Additionally, it is evident from Figure 7.5 that the flue gas temperature after the recuperator reaches 272°C, which is sufficient for the drying process.

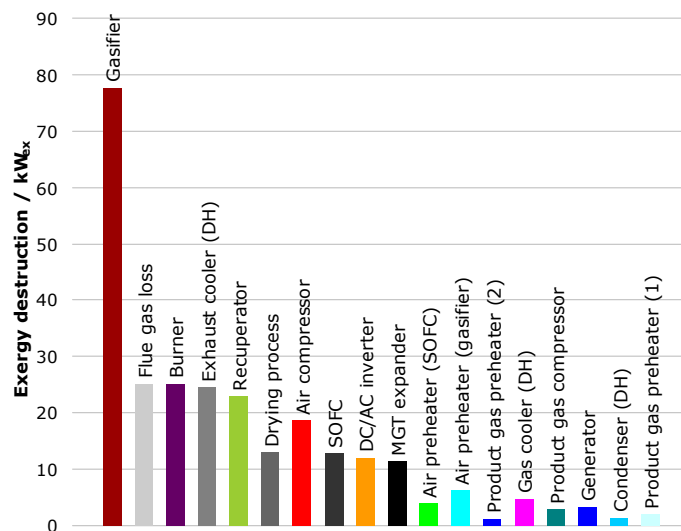


Figure 7.6: Exergy losses and destructions in the different components of the optimized SOFC-MGT plant configuration. Total exergy destruction and loss in the plant is approximately 269 kW_{ex} . The components are listed in the same order as in Figure 7.3.

It should be noted that some uncertainty is connected to the temperature of the product gas leaving the gasifier air preheater. This is due to the simplified model of the gasification process (combining pyrolysis, partial oxida-

tion, and char gasification in one component) and the temperature of the preheated gasifier air in the Viking gasifier, which is unknown to the author.

Figure 7.6 shows the exergy losses in the optimized SOFC-MGT system, and in Table 7.3, the changes in exergy destructions between the original and optimized scenarios are listed along with the exergy efficiencies of the components. The only new component is the first step product gas preheater. The total exergy loss in the optimized plant is approximately 269 kW_{ex}, around 17 kW_{ex} or 6% less than in the original case. Only components are listed in Table 7.3, so the change in exergy loss through the emitted flue gas is not included. Exergy lost in the flue gas loss is reduced by 6.0 kW_{ex} due to a reduced stack temperature.

The additional product gas preheater (first step) improves the performance of the original product gas preheater (second step) significantly (from $\eta_{\psi}=84.4\%$ to $\eta_{\psi}=92.0\%$). The total exergy destruction due to product gas preheating is reduced by 2.9 kW_{ex}, even though it is done in two components instead of one. The first step product gas preheater also improves the performance of the burner and MGT expander because of increased temperatures downstream the SOFCs. The exergy destruction in the burner is reduced to 25.2 kW_{ex} of which 13.9 kW_{ex} is due to mixing and 11.4 kW_{ex} is due to the irreversible combustion process. Of the exergy destruction caused by mixing, only 0.1 kW_{ex} is caused by thermal equilibration (13.8 kW_{ex} by diffusion). If compared to the contributions to the exergy destruction in the burner in the original SOFC-MGT system (described below Figure 7.3), the exergy destruction due to thermal equilibration is reduced by 1.8 kW_{ex} and due to the irreversible combustion process by 1.6 kW_{ex}. Thus, more equal temperatures of the burner inlets reduce the losses caused by the thermal equilibration, and the higher temperatures of the burner inlets reduce the losses caused by the combustion. The loss due to diffusion is the same as in the original scenario. The drying process is improved because the temperature differences in the steam heater are smaller. The reduced exergy destruction in the drying process of approximately 4.5 kW_{ex} is all due to improved steam heater performance.

Some components experience a greater exergy destruction in the optimized SOFC-MGT scenario than in the original one (e.g., the recuperator, compressors, MGT expander, and generator), but generally, all exergy efficiencies of the components either increase or are constant. The increased exergy destructions in some components originate from higher exergy inputs to the respective components and not reduced performance.

Table 7.3: Comparison of exergy destructions and exergy efficiencies^a of components from the original and optimized SOFC-MGT scenarios. The components are listed in order according to the exergy destructions in Figure 7.6.

Component	Change in exergy destruction / kW_{ex}	Original η_{ψ} / %	Optimized η_{ψ} / %
Gasifier	0.00	87.0	87.0
Burner	-3.45	93.1	94.7
Exhaust cooler (DH)	-2.17	32.6	36.3
Recuperator	2.06	86.2	86.9
Drying process ^b	-4.47	97.1	97.8
Air compressor	1.46	79.8	80.3
SOFC	-0.08	98.3	98.4
DC/AC inverter	0.03	95.0	95.0
MGT expander	1.12	93.6	94.0
Air preheater (SOFC)	-3.03	89.6	89.8
Air preheater (gasifier)	0.00	74.5	74.5
Product gas preheater (2)	-4.77	84.4	92.0
Gas cooler (DH)	-0.11	34.4	34.4
Product gas compressor	0.25	81.7	82.1
Generator	0.81	95.0	95.0
Condenser (DH)	0.00	90.1	90.1
Product gas preheater (1)	1.87 ^c	-	91.7 ^d

^a Inputs and products are defined in Table 7.1.

^b Includes dryer, steam blower, and steam heater (see Figure 5.3).

^c Equal to the absolute exergy destruction of this component in the optimized scenario because this component was not included in the original configuration.

^d Input: Exergy decrease of cooled product gas. Product: Exergy increase of heated product gas.

An additional optimization effort can be performed by introducing a first step preheater of the gasifier air, situated before the existing gasifier air preheater. This first step gasifier air preheater can be heated by the flue gas after the flue gas has heated the drying process and before the exhaust cooler. The temperature of the flue gas between the drying process and the exhaust cooler is 227°C. The cooling of the raw product gas in the second step air preheater will then be reduced and additional heat can be added to the pressurized product gas in the first step product gas preheater, thus increasing the product gas inlet to the burner, TIT, burner performance, and MGT expander performance. If this additional optimization suggestion is applied, the optimal *PR* increases slightly from 2.7 to 2.8, the TIT from 790°C to 802°C, and the net electrical efficiency from 58.2% to 58.6%. This is a relatively small performance gain when installing a first step gasifier air preheater compared to the introduction of a first step product gas preheater. Hence, this optimization effort is not documented in detail in this study. To find out if the latter suggested optimization is worth the effort, the increased revenue due to the small performance gain should be compared to the investment and maintenance costs of the additional heat exchanger and piping.

If costs were analyzed or a higher S/C ratio of the product gas was found necessary, removal of the condenser could be considered.

7.3 SUMMARY

1st and 2nd law analyses have been performed on the SOFC-MGT scenario revealing inefficiencies within the system. The gasifier reactor (including pyrolysis, partial oxidation, and char gasification) caused the greatest exergy destruction but still reached an exergy efficiency of 87%. Almost 28% of the total exergy loss in the plant took place in heat exchangers, 11% in turbomachineries, 10% in the burner, and 11% was lost via the flue gas leaving the plant. Exergy destruction attributable to the SOFCs only contributed to nearly 5% of the total exergy destruction in the plant, performing with an exergy efficiency of approximately 98%.

Assuming the plant components to be state-of-the-art, potential improvements of the system layout have been proposed and tested by additional process simulations. Improving the heat exchanger network by matching temperature levels showed to be beneficial, and the inclusion of a first step product gas preheater had a positive impact on several other components, e.g., the burner and MGT expander. All in all, the optimization effort only required the installation of one additional heat exchanger and still increased the performance of the SOFC-MGT plant substantially. The energetic net

electrical efficiency increased from 55.0% to 58.2% and the exergetic net electrical efficiency from 47.6% to 50.4%. Mainly, additional net power production from the MGT ensured the performance gain of the plant. In the optimized scenario, heat for drying the biomass was supplied by the exhaust from the SOFC-MGT subsystem instead of hot product gas from the gasifier reactor. Furthermore, the temperature of flue gas leaving the plant was reduced from 120°C to 90°C increasing the cogeneration efficiency from 82.6% to 87.5% based on energy and from 50.5% to 53.4% based on exergy.

Chapter 8 CONCLUDING REMARKS

The aim of this research was to contribute to enhanced electrical efficiencies and sustainability in future decentralized CHP plants. The work dealt with the coupling of thermal biomass gasification and SOFCs, and specific focus was kept on exploring the potential performance of hybrid CHP systems based on the novel two-stage gasification concept and SOFCs.

8.1 SUMMARY OF FINDINGS

Based on a review of existing literature, it was found essential to produce a clean product gas when aiming at electrochemical conversion in SOFCs. This showed to be partly obtainable by appropriate gasifier design and else by gas conditioning. The cleanliness of the product gas from the two-stage gasifier design ensured the need for only simple gas conditioning downstream the gasifier. For this reason, and high cold gas efficiency, the two-stage gasification concept was chosen for the studied plant scenarios.

Three conceptual plant designs were investigated in this study, all based on two-stage gasification of wood chips with a thermal biomass input of ~ 0.5 MW_{th} (LHV). The difference between the conceptual plant designs were the way of producing power and heat from the product gas from the gasification process. One scenario used a micro gas turbine (MGT), another SOFCs, and a third a combined SOFC and MGT system. The plant scenarios were investigated by system-level modelling combining zero-dimensional component models using the simulation software DNA. The modelled two-stage gasification process was calibrated against performance data from the demonstrated two-stage gasifier (Viking).

It was necessary to develop a new SOFC component model to predict the SOFC performance at various operating conditions. The SOFC component

model included an electrochemical model, which was calibrated against published data from Topsoe Fuel Cell A/S representing their 2nd generation SOFCs. A parametric study revealed the sensitivity of the SOFC performance to different operating conditions, and the results can be used as guidelines for optimal SOFC operation. At the reference conditions (300 mA cm⁻², 800°C, 1 bar, and 85% fuel utilization), the electric efficiency of the SOFCs reached 49% using product gas from two-stage biomass gasification. The SOFC performance showed to be slightly reduced compared to using hydrogen due to a lower hydrogen partial pressure. The parametric study also revealed a severe sensitivity of the SOFC performance to the SOFC operating temperature. Decreasing the temperature from the reference value of 800°C reduced the electrical SOFC efficiency significantly. Also, the fuel utilization greatly influenced the electrical SOFC efficiency and should be maintained at a high level, but the SOFC converted the *reacting* fuel to electricity equally efficient in the studied range of fuel utilizations, though. Hence, the fuel utilization could be changed, for reasons originating elsewhere in the system, without changing how efficiently the reacting fuel in the SOFC was converted to electricity. The SOFC performance only showed a moderate gain from increasing operating pressure, predominantly at low pressure.

From plant simulations, the performances and parametric tendencies of the studied plant configurations were investigated. Similar for all plant scenarios were the gasifier plant part performing with a cold gas efficiency of 94% and an exergy efficiency of 81%. The pressure ratio showed to be an important parameter in the two pressurized systems, revealing optimum values of 3.7 in the MGT scenario and 2.5 in the SOFC-MGT scenario with respect to the net electrical efficiencies of the plants. The turbine inlet temperature (TIT) should be maximized to enhance MGT performance, but was limited by a cold and lean burner feed in the SOFC-MGT scenario caused by the SOFC operation. The influence of turbomachinery performance was only significant in the two pressurized systems. Furthermore, it was found that for all three plant scenarios, the condenser, situated as the last step in the gasification plant part, could be removed without affecting the plant performances. Hereby, the plant complexities could be reduced, thus also the plant investment costs. Additionally, removal of the condenser would increase the steam-to-carbon (S/C) ratio of the product gas from 0.41 to 0.51, thus reducing the risk of carbon deposition in the SOFCs. Of the SOFC operating parameters important to the system performance, the SOFC operating temperature and fuel utilization was crucial. The SOFC operating temperature should be maintained at a high level to avoid both decreased SOFC performance and MGT performance. The latter caused by a lower TIT. The fuel utilization should also be maintained at a high level to ensure use of the most of the fuel in the SOFCs because of their superior electrical efficiency.

In the SOFC-MGT scenario, the SOFC fuel utilization could also be used to regulate the TIT, but still the optimal plant performance was at high fuel conversion in the SOFCs. Also the current density had great impact on the SOFC and system performances, but the choice of current density is an issue of SOFC dimensioning and should be evaluated from an economical viewpoint. A greater temperature difference across the cathode reduced the necessary mass flow of air to cool the SOFC, but in the SOFC scenario, this temperature difference did not have significant impact on the system performance because of the low influence of air compressor work when operating the SOFC at atmospheric pressure. Contrary in the SOFC-MGT scenario, the chosen temperature difference across the cathode should be maximized to keep a high TIT and system performance (limited by thermal stresses in the SOFCs).

At the optimal pressure ratio, the MGT scenario performed with a net electrical efficiency of 27% (LHV) and a cogeneration efficiency of 75% (LHV), producing 134 kW_e AC power and 240 kJ s⁻¹ of district heating. The corresponding exergy efficiencies were 23% and 28%, respectively. The SOFC plant scenario performed better than the MGT scenario reaching a net electrical efficiency of 43% (LHV) and a cogeneration efficiency of 83% (LHV), producing 215 kW_e AC power and 199 kJ s⁻¹ of district heating. The corresponding exergy efficiencies were 37% and 42%, respectively. The SOFC-MGT plant scenario showed the greatest potential performing with a net electrical efficiency of 55% (LHV) and a cogeneration efficiency of 83% (LHV) at the optimal pressure ratio. The AC power production reached 275 kW_e and the district heating production 138 kJ s⁻¹. The corresponding exergy efficiencies were 48% and 51%, respectively. The inclusion of a MGT in an SOFC system not only ensured a higher electrical efficiency, but also ensured less sensitivity of the electrical efficiency to the operating conditions of the SOFCs. At lower SOFC performance, the SOFCs produced less electricity but additional heat. The additional heat could be utilized by the MGT, though at a lower conversion efficiency. Generally, it can be stated that combining SOFCs with downstream heat engines ensures a higher system performance and a greater robustness to conditions causing varying SOFC performance. On the other hand, the SOFC-MGT scenario showed that higher system complexity limits the operational window of several parameters.

From 1st and 2nd law analyses, the SOFC-MGT scenario was optimized reaching a net electrical efficiency of 58% (LHV) and a cogeneration efficiency of 88% (LHV). The performance gain was ensured by an improved heat exchanger network and a decreased plant exhaust temperature. The additional power generation was produced by the MGT because the inclusion of a first step product gas preheater reduced exergy destructions in several

components and increased the TIT. All in all, the optimization effort only required the installation of one additional heat exchanger and still increased the performance of the SOFC-MGT plant substantially.

8.2 RECOMMENDATIONS FOR FURTHER WORK

8.2.1 SOFC COMPONENT MODEL

A zero-dimensional SOFC component model was developed for the DNA simulation tool in a FORTRAN environment. The SOFC model included an electrochemical model contributing to the prediction of the overall SOFC performance depending on operating conditions like temperature, pressure, fuel utilization, and gas compositions.

The data used for calibration could be improved. The active cell area in the dataset is not published in the open literature (confidential) forcing it to be assumed in this study. Hence, it was assumed to be 81 cm^2 per cell. A different active cell area would change the calibration and the SOFC performance. Therefore, a dataset with sufficient information would enable better calibration. With the assumed active cell area, the published dataset only covered a current density range from 0 to $\sim 220 \text{ mA cm}^{-2}$, and the reference operation point used in this study was 300 mA cm^{-2} . Hence, an extended dataset including high current density operation would improve the reliability of the calibrated SOFC component model, even though the polarization curve is almost linear from 220 to 300 mA cm^{-2} .

As discussed in Appendix J, CO should not be considered equal to H_2 nor inert when calculating the anodic exchange current density. It is suggested to find a more generic expression for the anodic exchange current density, and one approach is suggested in the end of Appendix J.

The concentration overpotential is caused by limitations of diffusive transport of reactants and products between the flow channel and the electrode-electrolyte interface. The effect is increasing with current density, and at a certain current density limit, this transport of species is not fast enough to feed the electrochemical reactions taking place. In the electrochemical model of the SOFCs, this limiting current density is assumed constant. In reality, the SOFC operating conditions and the microstructural characteristics of the electrodes will affect the limiting current density. Detailed models describing the limiting current density are available and could be implemented in the SOFC component model for better performance predictions at higher current densities.

Incorporating dependency of inlet temperatures to the predicted SOFC performance could be relevant. In the current SOFC component model, the temperature of the solid SOFC structure is assumed to be equal to the outlet temperature of the SOFCs. Thus, no negative effects of lower inlet temperatures, i.e., lower solid temperature and performance close to the inlets, are taken into account. The obvious approach would be to upgrade the model to be at least one-dimensional, but it could be interesting to investigate if use of an average temperature or the like is satisfactory, hence keeping the simplicity of zero-dimensional component models.

8.2.2 MODELLED GASIFICATION PROCESS

In the two-stage gasification concept, pyrolysis takes place in a separate reactor prior to the reactor where partial oxidation and char gasification occurs. Furthermore, the pyrolysis reactor is heated by the product gas leaving the gasification reactor. In the modelled gasification process, both pyrolysis, partial oxidation, and char gasification takes place in one gasifier component eliminating the potential for alternative thermal integration with that part of the gasification process. Still, the resulting product gas composition and cold gas efficiency are similar to those of the demonstrated two-stage gasifier. Development of a pyrolysis component model would improve the level of detail in the gasification process and enable investigation of additional process integration. Furthermore, access to temperature data of all inlets and outlets of the components in the demonstrated two-stage gasifier would enable better calibration of the modelled gasification process.

8.2.3 OPTIMIZATION EFFORTS

Besides the optimization efforts implemented in Chapter 7, additional ideas evolved during the progress of this study, unfortunately, without finding the time to test their potential. The ideas are listed below:

- *Methanation*

By including a methanation reactor (opposite of steam reforming, eq. (2.10)) prior to the SOFC anodes, the methane content in the product gas could be increased and internal reforming of the methane would contribute to the SOFC cooling. Hereby, the excess air flow on the cathode side could be decreased. Furthermore, the exothermic methanation process could eliminate the need for a product gas pre-heater (anode in/out heat exchanger), thereby ensuring a higher temperature of the product gas fed to the burner and a higher TIT. Water produced in the methanation process would also increase the S/C ratio, thus lowering the risk of carbon formation in the SOFCs.

- *Enriched air for gasifier*

The composition of the product gas from the gasifier contains a lot of N_2 (approximately one third on a dry volume basis). By reducing the N_2 content in the air fed to the gasifier, the N_2 content in the product gas would also be reduced. This could be done by membrane technology utilizing materials with O_2 permeability. Membranes can enrich air to the cost of pressurization (approximately 38% O_2 at 2 bar and 55% O_2 at 5 bar [78]). Thus, the system performance gain from a less N_2 -dilute product gas should cover the additional compressor work.

- *Cathode off gas recycling*

By cooling and recycling cathode off gas to the cathode inlet, the mass flow of air supplied by the air compressor could be reduced, and still, a high mass flow through the cathode could be maintained to ensure sufficient SOFC cooling. Proper utilization of the heat in the cathode off gas would be needed. By this method, the TIT could be increased and, at the same time, the size of the turbomachinery and recuperator could be reduced, thus lowering the investment costs. Nagel et al. [52] underlined that the air-to-fuel ratio is highly cost effective in such systems as it determines equipment size. Furthermore, the lower exhaust mass flow would reduce the exergy lost in the flue gas.

8.3 OUTLOOK

The thermodynamic potential of combining biomass gasification and efficient conversion of product gas in SOFCs to generate sustainable power and heat has been shown in this study. This was based on a developed SOFC component model, which the author hopes can contribute to many later studies of SOFC plants in general using DNA. A couple of projects concerning SOFC-based plants already use the developed SOFC component model.

The modelled scenarios in this study have aimed at the scale of the largest two-stage gasifier demonstrated today, $\sim 0.5 \text{ MW}_{th}$ (LHV). Thus, in the best and optimized scenario, the power output is only $\sim 0.3 \text{ MW}_e$. That is sufficient for very small decentralized CHP plants, but larger decentralized CHP plants in the size of 5-30 MW_e should also be investigated. A potential for even higher electrical efficiencies exists in these larger plants because of better turbomachinery at that scale. Steam-based Rankine cycles might also be relevant, e.g., heated by the gas turbine exhaust. The progress of upscal-

ing is also limited by the development of larger two-stage gasifiers. The two-stage gasification concept is claimed to be scalable up to 3-10 MW_{th} reaching even higher cold gas efficiency [15]. Alternatively, other gasifier types could be investigated, but high cold gas efficiency and clean product gas are vital.

The feasibility of a CHP plant is not only governed by its thermodynamic performance, but also investment and maintenance costs drive the competitiveness of a plant. Thus, economic issues should also be investigated before final conclusions can be made on the prospect of future CHP plants based on biomass gasification and SOFCs. Yet, it is difficult to predict the investment costs of novel gasifiers and SOFCs because they are not yet fully commercial. If reasonable estimates on future gasifier and SOFC prices are made, preliminary investigations of the economic feasibility can be performed. The method of thermoeconomics, applying the concept of cost to exergy, can be used to evaluate cost formations in the plant [76] [79].

Furthermore, issues like start-up strategy and dynamic behaviour, which were not considered in this study, can be very important issues when comparing plant performances.

A research project, aiming at long-term testing of SOFC operation on product gas from the demonstrated 75 kW_{th} two-stage gasifier, is under way. Based on the research in this study, evaluation of the long-term SOFC tests, and additional system analyses, the research project will make an assessment of the potential of combining two-stage biomass gasification and SOFCs. If the conclusion of the research project indicates a promising future for two-stage gasifier and SOFC couplings, later pilot scale demonstration is expected.

8.4 FINAL STATEMENT

An investigation of the potential performance of biomass gasification and SOFC hybrid systems for decentralized CHP production has been conducted. The investigation incorporated detailed component-level modelling of the SOFCs, system-level modelling of the complete process, and optimization of the plant layout. The two-stage gasification concept was found ideal for a high-efficient SOFC-based CHP plant due to its high cold gas efficiency and clean product gas. Besides ensuring the predicted SOFC performance to be dependent on the operating conditions, the SOFC component model was used to issue guidelines for optimal SOFC operation. A great potential for combined two-stage gasification and SOFC power generation was revealed. Net electrical plant efficiencies of 50-60% (LHV) was found

achievable when integrating gas turbine technology to utilize the SOFC off gases, thus establishing greater electric power yield compared to traditional decentralized CHP plants, which only achieve net electrical plant efficiencies of 30-34% (LHV) on biomass. Future experimental tests and demonstrations should verify the predicted potential presented in this study.

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Appendix A THE GIBBS FREE ENERGY MINIMIZATION METHOD

A chemical equilibrium is characterized by the fact, that the total Gibbs free energy of a system has its minimum value. This characteristic can be used to calculate the gas composition at chemical equilibrium, at specified temperature and pressure, without considering the reaction pathway of the chemical compounds involved. This Gibbs free energy minimization methodology is described in this appendix and is based on Smith et al. [58] and Elmegaard [56]. The Gibbs free energy minimization methodology was first described by White et al. [80].

Considering a gas mixture of k ideal gas compounds, the total Gibbs free energy of the system can be expressed as:

$$\dot{G}_{\text{tot}} = \sum_{i=1}^k \dot{n}_i [g_i^0 + RT \ln(y_i p)] \quad (\text{A.1})$$

\dot{n} being the molar flow, g^0 the molar specific standard Gibbs free energy, and y the molar fraction – all three for each gas compound. g^0 is only a function of temperature.

The minimum value of the expression for the total Gibbs free energy of the system should be found within the material balance constraints. The reacting compounds are not conserved in the system, but the total number of atoms of each chemical element⁴ should be preserved.

⁴ A chemical element is a chemical substance made up of one type of atom (e.g., H). A chemical compound (e.g., H₂ or CO₂) consists of more than one chemical element.

Considering a system with w chemical compounds entering into the system and k chemical compounds leaving the system at chemical equilibrium, the material balance can be expressed,

$$\begin{aligned} \sum_{v=1}^w \dot{n}_{v,\text{in}} A_{vj} &= \sum_{i=1}^k \dot{n}_{i,\text{out}} A_{ij}, \quad j = \{1, 2, \dots, N\} \Leftrightarrow \\ \sum_{i=1}^k \dot{n}_{i,\text{out}} A_{ij} - \sum_{v=1}^w \dot{n}_{v,\text{in}} A_{vj} &= 0, \quad j = \{1, 2, \dots, N\} \end{aligned} \quad (\text{A.2})$$

where A_{vj} is the number of atoms of element j in each molecule of entering compound v , A_{ij} is the number of atoms of element j in each molecule of leaving compound i . N is the total number of different chemical elements in the system. Eq. (A.2) describes the material constraints and consists of N equations, the unknown parameter being $\dot{n}_{i,\text{out}}$, one for each leaving chemical compound. Thus, k unknowns.

A Lagrange multiplier (λ) is introduced to each of the N material constraints, and the material constraints are summarized:

$$\begin{aligned} \lambda_j \left(\sum_{i=1}^k \dot{n}_{i,\text{out}} A_{ij} - \sum_{v=1}^w \dot{n}_{v,\text{in}} A_{vj} \right) &= 0, \quad j = \{1, 2, \dots, N\} \Leftrightarrow \\ \sum_{j=1}^N \lambda_j \left(\sum_{i=1}^k \dot{n}_{i,\text{out}} A_{ij} - \sum_{v=1}^w \dot{n}_{v,\text{in}} A_{vj} \right) &= 0 \end{aligned} \quad (\text{A.3})$$

Since eq. (A.3) is equal to zero, a new function, F , identical to \dot{G}_{tot} at the system outlet, can be defined as:

$$F = \dot{G}_{\text{tot,out}} + \sum_{j=1}^N \lambda_j \left(\sum_{i=1}^k \dot{n}_{i,\text{out}} A_{ij} - \sum_{v=1}^w \dot{n}_{v,\text{in}} A_{vj} \right) \quad (\text{A.4})$$

The function F is equal to $\dot{G}_{\text{tot,out}}$, but also incorporates the material constraints, and, as for $\dot{G}_{\text{tot,out}}$, the minimum value of F represents chemical equilibrium. To find the outlet gas composition at chemical equilibrium, the set of outlet molar flows, $\dot{n}_{i,\text{out}}$, should be chosen so the function F is at a minimum. F can be minimized by setting the partial derivatives of F , with respect to the molar flow of each outlet compound $\dot{n}_{i,\text{out}}$, equal to zero. Thus,

$$\begin{aligned} \frac{\partial F}{\partial \dot{n}_{i,\text{out}}} &= \frac{\partial \dot{G}_{\text{tot,out}}}{\partial \dot{n}_{i,\text{out}}} + \sum_{j=1}^N \lambda_j A_{ij} = 0, \quad i = \{1, 2, \dots, k\} \Leftrightarrow \\ g_{i,\text{out}}^0 + RT \ln(y_{i,\text{out}} p) + \sum_{j=1}^N \lambda_j A_{ij} &= 0, \quad i = \{1, 2, \dots, k\} \end{aligned} \quad (\text{A.5})$$

From eq. (A.5) a set of k equations are defined, one for each chemical compound leaving the system, the unknown parameters being $y_{i,\text{out}}$ and λ_j .

Since,

$$y_{i,\text{out}} = \frac{\dot{n}_{i,\text{out}}}{\sum_{i=1}^k \dot{n}_{i,\text{out}}}, \quad i = \{1, 2, \dots, k\} \quad (\text{A.6})$$

eq. (A.5) can be expressed by use of molar flows instead of molar fractions:

$$g_{i,\text{out}}^0 + RT \ln\left(\frac{\dot{n}_{i,\text{out}}}{\sum_{i=1}^k \dot{n}_{i,\text{out}}} p\right) + \sum_{j=1}^N \lambda_j A_{ij} = 0, \quad i = \{1, 2, \dots, k\} \quad (\text{A.7})$$

Then, eqs. (A.2) and (A.7) constitute N material balance equations and k equilibrium equations having N unknown Lagrange multipliers (λ_j) and k unknown outlet molar flows ($\dot{n}_{i,\text{out}}$). This system of $N+k$ equations with $N+k$ unknowns can readily be solved determining the outlet molar flows (and Lagrange multipliers), and the outlet gas composition can then be determined from eq. (A.6).

In the case of using the Gibbs free energy minimization method for calculating the outlet composition of the SOFC anode, as described in Chapter 4, the following chemical compounds and elements are included:

$$\begin{aligned} \text{Inlet:} \quad & v = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2, \text{O}_2\} \\ \text{Outlet:} \quad & i = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2\} \\ \text{Elements:} \quad & j = \{\text{H}, \text{C}, \text{O}, \text{N}\} \end{aligned}$$

Then, $k=6$ and $N=4$, resulting in a set of 10 equations with 10 unknowns. The O_2 is coming from the cathode side, and $\dot{n}_{\text{O}_2,\text{in}}$ can be found from eq. (4.6). Operating temperature and pressure of the SOFC are used in eq. (A.7).

In the case of using the Gibbs free energy minimization method for calculating the outlet composition of the gasifier, as described in Section 5.1.1, the following chemical compounds and elements are included:

$$\begin{aligned}\text{Inlet:} \quad & v = \{\text{C}_7\text{H}_7\text{O}_7, \text{H}_2\text{O}, \text{N}_2, \text{O}_2, \text{Ar}, \text{CO}_2\} \\ \text{Outlet:} \quad & i = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2, \text{Ar}, \text{H}_2\text{S}\} \\ \text{Elements:} \quad & j = \{\text{H}, \text{C}, \text{O}, \text{N}, \text{Ar}, \text{S}\}\end{aligned}$$

Then, $k=8$ and $N=6$, resulting in a set of 14 equations with 14 unknowns. The solid biomass composition is not defined here, but the composition used in the two-stage Viking gasifier can be found in Table 5.2. The ashes and additional methane (*METH*) are not included in the equilibrium calculations. Operating temperature and pressure of the gasifier are used in eq. (A.7).

Appendix B SOFC COMPONENT MODEL LISTING

Included in this Appendix are:

- SOFC component model code (11 pages)
- Flow sheet of SOFC component test with node numbers (1 page)
- DNA Input for SOFC component test (2 pages)
- DNA Output for SOFC component test (2 pages)

The input and output data only represent one simulation using the reference conditions.


```

1  C*****
2      SUBROUTINE SOFCEQ0D_CBM (KOMTY,ANTLK,ANTEX,ANTKN,ANTPK,ANTM1,
3      $      MEDIE,ANTME,VARME,ANTEL, VAREL,parnam,zanam
4      $      ,MDOT,P,H,E,Q,ZA,PAR,RES,X_J,KOMDSC,KMEDDS,K_PAR,K_LIG
5      $      ,K_BET,k_inp)
6  C*****
7  C
8  C  SOFCEQ0D_CBM is a model of a Solid Oxide Fuel Cell with outlet gas
9  C  composition based on chemical equilibrium. It is based on the simple
10 C  SOFCEQ_2 (BE 2004), so N2 can be used on the anode side.
11 C  The calculation of the reversible efficiency (ETAMAX) have been
12 C  corected and the voltage efficiency is calculated by an
13 C  electrochemical model based on the operating conditions instead of
14 C  being an input parameter.
15 C*****
16 C
17 CA FKOMP - INPUT - Flag with the value:
18 CA          1: Initialize the component.
19 CA          2: Initialize with actual system.
20 CA          3: Fluid composition calculation (constant).
21 CA          4: Find residuals.
22 CA          5: Find residuals and check variables.
23 CA          6: Output information about component.
24 CA MDOT - INPUT - Massflows from nodes.
25 CA P - INPUT - Pressure in nodes.
26 CA X_J - INPUT - Fluid composition.
27 CA KOMTY - OUTPUT - Component name.
28 CA ANTPK - OUTPUT - Number of parameters for the component.
29 CA ANTLK - OUTPUT - Number of equations in the component.
30 CA ANTEX - OUTPUT - Number of independent equations in the component.
31 CA ANTED - OUTPUT - Number of differential independent equations.
32 CA ANTKN - OUTPUT - Number of nodes connected to the component.
33 CA ANTM1 - OUTPUT - Number of massflows in the first conservation of
34 CA          mass equation.
35 CA ANTM2 - OUTPUT - Number of massflows in the second.
36 CA DYCOM - OUTPUT - Type of conservation equations (static or dynamic
37 CA          mass and internal energy on side 1 and 2 respectively;
38 CA          and dynamic solid internal energy).
39 CA MEDIE - IN/OUT - Media (fluid) of the connected nodes.
40 CA          The values mean :
41 CA          -4 : Any gas
42 CA ANTME - OUTPUT - Number of fluids with variable composition.
43 CA VARME - OUTPUT - Pointer to fluid numbers (with variable composition).
44 CA ANTEL - OUTPUT - Number of computed compounds in these variable fluids.
45 CA VAREL - OUTPUT - Compound numbers in variable fluids.
46 CA RES - OUTPUT - Residuals for the component.
47 C
48 C  ANTST - Number of fluid compounds in DNA.
49 C
50 CL XMIX  Composition of the mixture.
51 CL K_PAR Parameter description.
52 CL K_LIG Equation description.
53 CL K_BET Condition description.
54 CL K_MED Media description.
55 C
56 C  Subroutines : COMINF
57 C
58 C
59 CP Programmer: Christian Bang-Møller (CBM), TES, MEK, DTU, 2010
60 C*****
61
62 C  Including the common "environment"
63 C      INCLUDE 'ENVIRO.INI'
64 C      INCLUDE 'THERPROP.DEC'
65 C      INCLUDE 'GASI.DEC'
66 C
67 C  Parameter variables
68 C      INTEGER      ANTLK, ANTEX, ANTKN, MEDIE(6), ANTPK,
69 C      :            ANTM1, ANTME, VARME(4), ANTEL(4),
70 C      :            VAREL(ANTST,4)
71 C      DOUBLE PRECISION X_J(MAXME,ANTST),RES(39),MDOT(4),P(4),H(4),
72 C      :            E,Q,PAR(7),ZA(22)
73 C      CHARACTER*3     DYCOM(5)
74 C      CHARACTER*80     KOMTY,PARNAM(7),ZANAM(22)
75 C
76 C  Local variables

```

```

77     INTEGER I,J
78     DOUBLE PRECISION NIN(ANTST+1),NOUT(ANTST+1),ETASYS,G(6),HG(6),R,
79     $      M_BR_OUT,M_AIR_OUT,T3,T4,TGAS,ETAPRO,U,V,S,X,DUM,
80     $      M_BL(4),NO2IN,NH2IN,DP1,DP2,PGAS,UF,ETAMAX,T0,GMAX,
81     $      DT,i_load,eta_DCAC,F,n_e,i_n,STCR,
82     $      p_anode,p_cathode,p_H2,p_H2eq,p_CO,p_CH4,p_CO2,p_H2O,p_O2,
83     $      p_N2,p_H2Opr,
84     $      V_cell,
85     $      E_ernst,p_standard,G_s(3),G_standard,G2(5),G_real,
86     $      V_act,V_act_a,V_act_c,c_a,c_c,i_0_a_0,i_0_c_0,i_0_a,i_0_c,
87     $      gamma_a,gamma_c,E_act_a,E_act_c,i_0_a2,i_0_c2,i_0_a3,
88     $      V_ohm,sigma_e_0,E_act_e,sigma_e,delta_e,R_e,
89     $      V_conc,i_as,
90     $      n_ptot_FO,p_pCO2_FO,p_pH2O_FO,p_O2_FO,G_O2_FO,G_pCO2_FO,
91     $      G_pH2O_FO,GO2
92
93     CHARACTER*100      K_PAR(7)
94     CHARACTER*500      K_LIG(23), K_BET, KOMDSC
95     character*1000      K_INP
96     CHARACTER*100      KMEDDS(6)
97     EXTERNAL            COMINF
98     INCLUDE 'THERPROP.INI'
99     INCLUDE 'GASI.INI'
100
101 C=====
102     GOTO (200,200,1,400,400,200) FKOMP
103 1     RETURN
104 C-----
105 C  Component name
106 C-----
107 c 100 CONTINUE
108 c      KOMTY      = 'SOFCEQ0D_CBM'
109 c      GOTO 9999
110 C-----
111 C  Component characteristics
112 C-----
113 200 CONTINUE
114     KOMTY      = 'SOFCEQ0D_CBM'
115     ANTKN      = 6
116     ANTPK      = 7
117     ANTLK      = 17
118     ANTEX      = 23
119     ANTM1      = 4
120     MEDIE(1)   = anygas$
121     MEDIE(2)   = anygas$
122     MEDIE(3)   = anygas$
123     MEDIE(4)   = anygas$
124     MEDIE(5)   = power$
125     MEDIE(6)   = heat$
126     ANTME      = 4
127     VARME(1)   = NODE1$
128     ANTEL(1)   = 0
129     VARME(2)   = NODE2$
130     ANTEL(2)   = 0
131     VARME(3)   = NODE3$
132     ANTEL(3)   = 6
133     VARME(4)   = NODE4$
134     ANTEL(4)   = 5
135     VAREL(1,3) = H2$
136     VAREL(2,3) = CO$
137     VAREL(3,3) = CO2$
138     VAREL(4,3) = H2O_g$
139     VAREL(5,3) = CH4$
140     VAREL(6,3) = N2$
141     VAREL(1,4) = O2$
142     VAREL(2,4) = N2$
143     VAREL(3,4) = CO2$
144     VAREL(4,4) = H2O_g$
145     VAREL(5,4) = AR$
146     ZANAM(1)   = 'MULTIPLIER H'
147     ZANAM(2)   = 'MULTIPLIER C'
148     ZANAM(3)   = 'MULTIPLIER N'
149     ZANAM(4)   = 'MULTIPLIER O'
150     ZANAM(5)   = 'GIBBS ENERGY'
151     ZANAM(6)   = 'ETAMAX'
152     ZANAM(7)   = 'ETASYS'

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153     ZANAM(8) = 'UF'
154     ZANAM(9) = 'ETATOT'
155     ZANAM(10) = 'STCR'
156     ZANAM(11) = 'E_nernst'
157     ZANAM(12) = 'V_act'
158     ZANAM(13) = 'V_ohm'
159     ZANAM(14) = 'V_conc'
160     ZANAM(15) = 'V_cell'
161     ZANAM(16) = 'GMAX'
162     ZANAM(17) = 'G(T)'
163     ZANAM(18) = 'G(p,T)'
164     ZANAM(19) = 'p_H2eq'
165     ZANAM(20) = 'R_e'
166     ZANAM(21) = 'i_load'
167     ZANAM(22) = 'eta_DCAC'
168
169     PARNAM(1) = 'FUEL UTILIZATION'
170     PARNAM(2) = 'TGAS'
171     PARNAM(3) = 'DP FUEL'
172     PARNAM(4) = 'DP AIR'
173     PARNAM(5) = 'DT OUTLETS'
174     PARNAM(6) = 'Current density'
175     PARNAM(7) = 'DC/AC conversion efficiency'
176
177     IF (FKOMP.EQ.6) GOTO 600
178     ***     FKOMP = 3
179     GOTO 9999
180 C-----
181 C   Component equations. All in residual form.
182 C   Do not include the conservation laws, since these are treated
183 C   automatically by DNA.
184 C-----
185     400 CONTINUE
186     VAREL(1,3)=H2$
187     VAREL(2,3)=CO$
188     VAREL(3,3)=CO2$
189     VAREL(4,3)=H2O_G$
190     VAREL(5,3)=CH4$
191     VAREL(6,3)=N2$
192
193     UF=PAR(1)
194     TGAS=PAR(2)
195     DP1=PAR(3)
196     DP2=PAR(4)
197     DT=PAR(5)
198 C   (DT: Optional temperature difference between anode and cathode outlets)
199     i_load=PAR(6)
200     eta_DCAC=PAR(7)
201
202     R      = 8.314D0
203     T0     = 298.15D0
204     PGAS   = P(3)
205
206 C Pressure losses
207     RES(1) = P(1)-DP1-P(3)
208     RES(2) = P(2)-DP2-P(4)
209     p_anode=(P(1)+P(3))/2
210     p_cathode=(P(2)+P(4))/2
211
212 C Temperature of outlet gases
213 C (Anode outlet temperature equals TGAS)
214     CALL STATES(P(3),H(3),T3,V,S,X,DUM,1,2,MEDIE(3))
215     CALL STATES(P(4),H(4),T4,V,S,X,DUM,1,2,MEDIE(4))
216     RES(3) = T3-T4-DT
217     RES(4) = T3-TGAS
218
219 C Molar mass of the gases [kg/kmol]
220     M_BL(1)=0.D0
221     M_BL(2)=0.D0
222     M_BL(3)=0.D0
223     M_BL(4)=0.D0
224     DO I=1,ANTST
225         M_BL(1)=X_J(MEDIE(1),I)*M_MOL(I)+M_BL(1)
226         M_BL(2)=X_J(MEDIE(2),I)*M_MOL(I)+M_BL(2)
227         M_BL(3)=X_J(MEDIE(3),I)*M_MOL(I)+M_BL(3)
228         M_BL(4)=X_J(MEDIE(4),I)*M_MOL(I)+M_BL(4)

```

```

229         ENDDO
230
231 C Calculate mole flow of each species in to the reaction (used for Gibbs mini)
232 C (species in the anode inlet)
233     NIN(ANTST+1)=0.D0
234     DO I=1,ANTST
235         NIN(I)=MDOT(1)*X_J(MEDIE(1),I)/M_BL(1)
236         NIN(ANTST+1)=NIN(ANTST+1)+NIN(I)
237     ENDDO
238
239 C The available hydrogen (after steam reforming and water gas shift)
240     NH2IN=NIN(H2$)+NIN(CO$)+4*NIN(CH4$)
241 C Consumed oxygen
242 C (UF is defined so the actual hydrogen consumption is UF*NH2IN)
243 C (UF affects the Gibbs free energy minimization through the amount of consumed oxygen)
244     NO2IN=UF*NH2IN/2
245     NIN(O2$)=NIN(O2$)+NO2IN
246
247 C Flow of used air
248     RES(5) = MDOT(2)+MDOT(4)-NO2IN*M_MOL(O2$)
249 C Composition of used air
250     RES(6) = MDOT(2)/M_BL(2)*X_J(MEDIE(2),O2$)-NO2IN+
251     $ MDOT(4)/M_BL(4)*X_J(MEDIE(4),O2$)
252     RES(7) = MDOT(2)/M_BL(2)*X_J(MEDIE(2),N2$)+
253     $ MDOT(4)/M_BL(4)*X_J(MEDIE(4),N2$)
254     RES(8) = MDOT(2)/M_BL(2)*X_J(MEDIE(2),CO2$)+
255     $ MDOT(4)/M_BL(4)*X_J(MEDIE(4),CO2$)
256     RES(9) = MDOT(2)/M_BL(2)*X_J(MEDIE(2),H2O_G$)+
257     $ MDOT(4)/M_BL(4)*X_J(MEDIE(4),H2O_G$)
258     RES(10) = 1.D0-X_J(MEDIE(4),O2$)-X_J(MEDIE(4),N2$)-
259     $ X_J(MEDIE(4),CO2$)-X_J(MEDIE(4),H2O_G$)-
260     $ X_J(MEDIE(4),AR$)
261
262 C Calculate mole flow of each species out from the reaction (used for Gibbs mini)
263 C (species in the anode outlet)
264     NOUT(ANTST+1)=0.D0
265     DO I=1,ANTST
266         NOUT(I)=(-MDOT(3))*X_J(MEDIE(3),I)/M_BL(3)
267         NOUT(ANTST+1)=NOUT(ANTST+1)+NOUT(I)
268     ENDDO
269
270
271
272 C -----
273 C Start---Calculation of anode outlet composition from Gibbs free energy minimization-----
274 C -----
275 C Gibbs free energy of each compound
276 C (at outlet and without oxygen)
277     CALL STATES(P(3),H(3),TGAS,V,S,X,U,1,2,MEDIE(3))
278     TGAS = TGAS+273.15D0
279
280     DO I=1,6
281         CALL GIBBS(VAREL(I,3),TGAS,P(3)*X_J(MEDIE(3),VAREL(I,3)),G(I))
282     ENDDO
283
284     CALL GIBBS(O2$,TGAS,P(3)*X_J(MEDIE(3),O2$),GO2)
285
286 C Partial derivatives of the function to be minimized with respect to
287 C each species molar fraction
288     DO I=1,6
289         RES(I+10)=G(I)
290         DO J=1,4
291             RES(I+10) = RES(I+10) + ZA(J)*EL(VAREL(I,3),J)
292         ENDDO
293     ENDDO
294
295 C Molar balance for each atom (H,C,N)
296 C O balance is substituted by summation of molar fractions
297     DO J=1,3
298         RES(16+J) = 0.D0
299         DO I=1,ANTST
300             RES(16+J)=RES(16+J)-(NIN(I)-NOUT(I))*EL(I,J)
301         ENDDO
302     ENDDO
303     RES(20)=1.D0
304     DO I=1,ANTST

```

```

305         RES(20) = RES(20) - X_J(MEDIE(3), I)
306     ENDDO
307
308 C Summation of total Gibbs free energy of the considered species
309 C (H2, CO, CO2, H2O, CH4, N2 at anode outlet)
310     RES(21) = ZA(5)
311     DO I=1,6
312         RES(21) = RES(21) - G(I) * X_J(MEDIE(3), VAREL(I,3))
313     ENDDO
314 C -----
315 C End-----Calculation of anode outlet composition from Gibbs free energy minimization-----
316 C -----
317
318
319
320 C -----
321 C Start-----Calculating VOLTAGE EFFICIENCY (ETASYS) based on polarization losses-----
322 C -----
323 C     CONSTANTS
324 C     The universal gas constant (R) is already given above
325 C     Faradays constant [C/mol]:
326 C     F=96485
327 C     Number of moles of transferred electrons, n_e [mol e-/mol fuel (H2eq)]:
328 C     (equal to 2 since H2 (equivalent) is the only fuel in this electrochemical model,
329 C     [H. Zhu & R.J. Kee, J Power Sources 117 (2003) 61-74])
330 C     n_e=2
331 C     Internal current density [mA/cm^2]:
332 C     (mixed potential and fuel crossover) (used for calibrating OCV)
333 C     i_n=6
334
335
336 C     PARTIAL PRESSURES (AVERAGE)
337 C     Partial pressures before internal reforming [bar]:
338 C     (average between inlet and outlet)
339 C     p_H2 = (X_J(MEDIE(1), H2$) + X_J(MEDIE(3), H2$)) / 2 * p_anode
340 C     p_CO = (X_J(MEDIE(1), CO$) + X_J(MEDIE(3), CO$)) / 2 * p_anode
341 C     p_CO2 = (X_J(MEDIE(1), CO2$) + X_J(MEDIE(3), CO2$)) / 2 * p_anode
342 C     p_H2O = (X_J(MEDIE(1), H2O_G$) + X_J(MEDIE(3), H2O_G$)) / 2 * p_anode
343 C     p_CH4 = (X_J(MEDIE(1), CH4$) + X_J(MEDIE(3), CH4$)) / 2 * p_anode
344 C     p_N2 = (X_J(MEDIE(1), N2$) + X_J(MEDIE(3), N2$)) / 2 * p_anode
345 C     p_Ar = (X_J(MEDIE(1), Ar$) + X_J(MEDIE(3), Ar$)) / 2 * p_anode
346 C     p_O2 = (X_J(MEDIE(2), O2$) + X_J(MEDIE(4), O2$)) / 2 * p_cathode
347
348 C     Equivalent hydrogen partial pressure after internal reforming and
349 C     before anode reaction [bar]:
350 C     (derived from steam reforming and shift reactions)
351 C     p_H2eq = p_H2 + p_CO + 4 * p_CH4
352
353 C     Partial pressure of water product [bar]:
354 C     p_H2Opr = p_H2O
355
356
357 C     NERNST POTENTIAL
358 C     (based on [H. Zhu & R.J. Kee, J Power Sources 117 (2003) 61-74])
359
360 C     Change in Gibbs free energy of formation [J/mol]:
361 C     (G_standard is for hydrogen conversion at standard pressure and operating temp,
362 C     [S.C. Singhal & K. Kendall, High-Temperature Solid Oxide Fuel Cells: Fundamentals,
363 C     Design and Application (2003), p. 60])
364 C     p_standard = 1
365 C     CALL GIBBS(H2$, TGAS, p_standard, G_s(1))
366 C     CALL GIBBS(O2$, TGAS, p_standard, G_s(2))
367 C     CALL GIBBS(H2O_G$, TGAS, p_standard, G_s(3))
368 C     G_standard = G_s(3) - G_s(1) - 0.5 * G_s(2)
369 C     (G_real is for hydrogen conversion at average partial pressures and
370 C     operating temperature)
371 C     G_real = G_standard - R * TGAS * log(p_H2eq * sqrt(p_O2) / p_H2Opr)
372
373 C     Nernst potential - ideal voltage [V]:
374 C     E_nernst = (-G_real) / (n_e * F)
375
376
377 C     ACTIVATION OVERPOTENTIAL
378 C     (based on [S.H. Chan et al., J Power Sources 93 (2001) 130-140, eq. 9],
379 C     [H. Zhu & R.J. Kee, J Power Sources 117 (2003) 61-74],
380 C     and [T. Aloui & K. Halouani, Appl Thermal Eng 27 (2007) 731-737, eq. 8])

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381
382 C      Exchange current densities [mA/cm^2] based on [Costamagna & Honegger,
383 C      J. Electrochim. Soc., Vol. 145, No. 11 (1998) 3995-4007, table 3 and eq. 7+8]:
384 C      (eq. 7 is based on [Mogensen and Lindegaard, Solid Oxide Fuel Cells III (1993) 484])
385 C      (eq. 8 is based on [Achenbach, J Power Sources 49 333 (1994)])
386 C      (Ni/YSZ anode and LSM cathode)
387      gamma_a=2*5.5D9
388      gamma_c=0.5*7.0D8
389      E_act_a=1.2D5
390      E_act_c=1.2D5
391      i_0_c=gamma_c*(p_O2/p_cathode)**0.25*exp(-E_act_c/(R*TGAS))
392      i_0_a=gamma_a*(p_H2eq/p_anode)*(p_H2Opr/p_anode)*
393 $      exp(-E_act_a/(R*TGAS))
394 C      Eq. 6 from [Costamagna & Honegger] based on Yamamura:
395 C      i_0_a3=3.5*2.9D7*(p_H2eq/p_anode)*(p_H2Opr/p_anode)**(-0.5)*
396 C      $      exp(-E_act_a/(R*TGAS))
397
398 C      Exchange current densities [mA/cm^2] based on [Zhu & Kee]:
399 C      Anode exchange current density constant:
400 C      (used to calibrate activation overpotential)
401 C      i_0_a_0=5000
402 C      Cathode exchange current density constant (table 2 in [Zhu & Kee]):
403 C      (LSM-YSZ cathode)
404 C      i_0_c_0=750
405 C      Correlations based on eq. 29 in [Zhu & Kee]:
406 C      i_0_a2=i_0_a_0*(p_H2eq/p_anode)
407 C      i_0_c2=i_0_c_0*(p_O2/p_cathode)**0.5
408
409 C      Activation overpotential (eq. 33d+33e in [Chan]):
410 C      [arcsinh(x)=ln(x+sqrt(x^2+1))]
411      c_a=(i_load+i_n)/(2*i_0_a)
412      V_act_a=2*R*TGAS/(F)*log(c_a+sqrt(c_a**2+1))
413      c_c=(i_load+i_n)/(2*i_0_c)
414      V_act_c=2*R*TGAS/(F)*log(c_c+sqrt(c_c**2+1))
415      V_act=V_act_a+V_act_c
416
417 C      Alternative activation overpotential method:
418 C      (based on [J. Larminie & A. Dicks, Fuel cell systems explained (2003), p. 52]
419 C      and [F. Calise et al. Energy 31 (2006) 3278-3299])
420 C      From table 2 in [Calise]:
421 C      gamma_a=2.13D7
422 C      gamma_c=1.49D7
423 C      E_act_a=1.1D5
424 C      E_act_c=1.1D5
425 C      alpha_a=0.5
426 C      alpha_c=0.5
427 C      Internal current density [mA/cm^2] (mixed potential) (table 2 in [Calise]):
428 C      i_n=2
429 C      Exchange current densities (eq. 10+11 in [Calise]) [mA/cm^2]:
430 C      i_0_a=gamma_a*(p_H2eq/p_anode)*(p_H2Opr/p_anode)*
431 C      $      exp(-E_act_a/(R*TGAS))
432 C      i_0_c=gamma_c*(p_O2/p_cathode)**0.25*exp(-E_act_c/(R*TGAS))
433 C      Summation of anode and cathode overpotential (p. 52 in [Larminie] and
434 C      eq. 12+13 in [Calise]):
435 C      A_act_a=R*TGAS/(n_e*alpha_a*F)
436 C      A_act_c=R*TGAS/(n_e*alpha_c*F)
437 C      V_act=0.5*(A_act_a+A_act_c)*log((i_load+i_n)/(i_0_a*(A_act_a/
438 C      $      (A_act_a+A_act_c))+i_0_c*(A_act_c/(A_act_a+A_act_c))))
439 C      (0.5 is a calibration factor)
440
441
442 C      OHMIC OVERPOTENTIAL
443 C      Method by [H. Zhu & R.J. Kee, J Power Sources 117 (2003) 61-74]:
444 C      (ohmic resistance in an SOFC is typically dominated by ion resistance through the
445 C      electrolyte, thus the contributions from the electrodes and interconnects are neglected)
446 C      (based on a YSZ electrolyte)
447 C      Pre-factor of ionic conductivity [S*K/cm, S=ohm^(-1)], table 2 in [Zhu & Kee]:
448      sigma_e_0=3.6D5
449 C      Activation energy of transport of oxygen ions [J/mol], table 2 in [Zhu & Kee]:
450      E_act_e=8.0D4
451 C      Ionic conductivity of the electrolyte [S/cm or Ohm^(-1)*cm^(-1)], eq. 33 in [Zhu & Kee]:
452      sigma_e=sigma_e_0/TGAS*exp(-E_act_e/(R*TGAS))
453
454 C      Electrolyte thickness [cm]:
455 C      [S. Linderth et al., Materials Science Forum Vols. 539-543 (2007) 1309-1314, p. 1310]
456      delta_e=10D-4

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457
458 C      Area specific ohmic resistance of the electrolyte [Ohm*cm^2], eq. 34 in [Zhu & Kee]:
459 R_e=delta_e/sigma_e
460
461 C      Ohmic polarization losses [(mA/cm^2)*(Ohm*cm^2)/1000=V]
462 V_ohm=(i_load+i_n)*R_e/1000
463
464 C      Method by [S.H. Chan et al., Journal of Power Sources 103 (2002) 188-200, eq. 13-15 +
465 C      table 3] and [Bessette et al., Journal of Electrochemical Society, Vol. 142,
466 C      No. 11 (1995), table 1]:
467 C      Coefficients:
468 C          a_ohm_a=0.00298
469 C          b_ohm_a=-1392
470 C          a_ohm_c=0.00811
471 C          b_ohm_c=600
472 C          a_ohm_e=0.00294
473 C          b_ohm_e=10350
474 C          a_ohm_i=0.1256
475 C          b_ohm_i=4690
476 C      Layer thicknesses [cm]:
477 C      [S.H. Chan et al., Journal of Power Sources 93 (2001) 130-140, table 1]
478 C      (anode supported cell)
479 C          delta_a=750D-4
480 C          delta_c=50D-4
481 C          delta_e=40D-4
482 C      [S.H. Chan et al., Journal of Power Sources 103 (2002) 188-200, table 3]
483 C          delta_i=100D-4
484 C      Area specific resistance - ASR=[Ohm*cm^2]:
485 C          rho_a=a_ohm_a*exp(b_ohm_a/TGAS)
486 C          r_a=delta_a*rho_a
487 C          rho_c=a_ohm_c*exp(b_ohm_c/TGAS)
488 C          r_c=delta_c*rho_c
489 C          rho_e=a_ohm_e*exp(b_ohm_e/TGAS)
490 C          r_e=delta_e*rho_e
491 C          rho_i=a_ohm_i*exp(b_ohm_i/TGAS)
492 C          r_i=delta_i*rho_i
493 C          ASR=0.75*(r_a+r_c+r_e+r_i)
494 C          (0.75 is a calibration factor)
495
496
497 C      CONCENTRATION OVERPOTENTIAL
498 C      Method by [Kim, J.W. et al., J Electrochem Soc, 146 (1) (1999) 69-78]
499 C      and [Braun, R., Optimal Design and Operation of SOFC Systems for Small-scale Stationary
500 C      Applications (PhD thesis) (2002), eq. 4.8]:
501 C      (for anode-supported SOFCs i_cs>>i_as and the cathode concentration overpotential is
502 C      neglected)
503 C      Limiting current density of anode [mA/cm^2]:
504 C      (here assumed to be constant)
505 C          i_as=1000
506 C      Concentration overpotential [V]:
507 V_conc=-R*TGAS/(n_e*F)*(log(1-(i_load+i_n)/i_as)-
508 $      log(1+(p_H2eq*(i_load+i_n))/(p_H2Opr*i_as)))
509
510 C      Method by [F. Calise et al., Energy 31 (2006) 3278-3299, eq. 20]:
511 C      Limiting current density [mA/cm^2]:
512 C          i_l=900
513 C          V_conc2=-R*TGAS/(n_e*F)*log(1-(i_load+i_n)/i_l)
514
515
516 C      SINGLE CELL POTENTIAL
517 V_cell=E_nernst-V_act-V_ohm-V_conc
518
519
520 C      VOLTAGE EFFICIENCY
521 ETASYS=V_cell/E_nernst
522 C -----
523 C End-----Calculating VOLTAGE EFFICIENCY (ETASYS) based on polarization losses-----
524 C -----
525
526
527 C -----
528 C Start-----Calculating REVERSIBLE EFFICIENCY (ETAMAX)-----
529 C -----
530 C The reversible efficiency is the ratio between the change in Gibbs free energy of formation
531 C and the change in enthalpy of formation (here LHV) at full oxidation of the inlet fuel.
532 C [Zhu, H. and Kee, R.J., J Power Sources 161 (2006), p. 958]

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533
534 C Gibbs free energy of the reactants
535 C (based on partial pressures at inlet and SOFC operating temperature)
536 CALL GIBBS (H2$, TGAS, P(1) * X_J (MEDIE (1), H2$), G2 (1))
537 CALL GIBBS (CO$, TGAS, P(1) * X_J (MEDIE (1), CO$), G2 (2))
538 CALL GIBBS (CO2$, TGAS, P(1) * X_J (MEDIE (1), CO2$), G2 (3))
539 CALL GIBBS (H2O_G$, TGAS, P(1) * X_J (MEDIE (1), H2O_G$), G2 (4))
540 CALL GIBBS (CH4$, TGAS, P(1) * X_J (MEDIE (1), CH4$), G2 (5))
541
542 C Gibbs free energy of the stoichiometric amount of oxygen at Full Oxidation (FO)
543 C (considering the following 6 species: H2, CO, CH4, CO2, H2O, and N2)
544 p_O2_FO = (0.5 * X_J (MEDIE (1), H2$) + 0.5 * X_J (MEDIE (1), CO$) +
545 $ 2 * X_J (MEDIE (1), CH4$)) * P (1)
546 CALL GIBBS (O2$, TGAS, p_O2_FO, G_O2_FO)
547
548 C Partial pressure and Gibbs free energy of the products CO2 and H2O at Full Oxidation (FO)
549 C (considering the following 6 species: H2, CO, CH4, CO2, H2O, and N2)
550 n_ptot_FO = NIN (CO$) + 3 * NIN (CH4$) + NIN (CO2$) + NIN (H2$) + NIN (H2O_G$) +
551 $ NIN (N2$)
552 p_pCO2_FO = (NIN (CO$) + NIN (CH4$) + NIN (CO2$)) / n_ptot_FO * P (3)
553 p_pH2O_FO = (NIN (H2$) + 2 * NIN (CH4$) + NIN (H2O_G$)) / n_ptot_FO * P (3)
554 CALL GIBBS (CO2$, TGAS, p_pCO2_FO, G_pCO2_FO)
555 CALL GIBBS (H2O_G$, TGAS, p_pH2O_FO, G_pH2O_FO)
556
557 C Maximum change in Gibbs free energy at Full Oxidation (FO) [J/mol]
558 C (based on partial pressures at inlet for reactants and outlet for products)
559 C (considering the following 6 species: H2, CO, CH4, CO2, H2O and N2. Here N2 balances out)
560 GMAX = ((NIN (CO$) + NIN (CH4$) + NIN (CO2$)) * G_pCO2_FO +
561 $ (NIN (H2$) + 2 * NIN (CH4$) + NIN (H2O_G$)) * G_pH2O_FO -
562 $ NIN (H2$) * G2 (1) - NIN (CO$) * G2 (2) - NIN (CH4$) * G2 (5) -
563 $ NIN (CO2$) * G2 (3) - NIN (H2O_G$) * G2 (4) -
564 $ (0.5 * NIN (H2$) + 0.5 * NIN (CO$) + 2 * NIN (CH4$)) * G_O2_FO)
565 $ / NIN (ANTST + 1)
566
567 C Reversible efficiency (deltaG/deltaH)
568 ETAMAX = (-GMAX) /
569 $ (NED_H (H2$) * X_J (MEDIE (1), H2$) +
570 $ NED_H (CO$) * X_J (MEDIE (1), CO$) +
571 $ NED_H (CH4$) * X_J (MEDIE (1), CH4$))
572 C -----
573 C End-----Calculating REVERSIBLE EFFICIENCY (ETAMAX)-----
574 C -----
575
576
577 C Relation between power and heat loss
578 C (eta_DCAC is added to account for DC to AC conversion losses)
579 RES (22) = E + (NED_H (H2$) * NIN (H2$) + NED_H (CO$) * NIN (CO$) +
580 $ NED_H (CH4$) * NIN (CH4$)) * ETAMAX * ETASYS * UF * eta_DCAC
581
582 C Steam to carbon ratio at anode inlet
583 STCR = X_J (MEDIE (1), H2O_G$) /
584 $ (X_J (MEDIE (1), CH4$) + X_J (MEDIE (1), CO$) + X_J (MEDIE (1), CO2$))
585
586 C Printing of relevant variables
587 RES (23) = ZA (6) - ETAMAX
588 RES (24) = ZA (7) - ETASYS
589 RES (25) = ZA (8) - UF
590 RES (26) = ZA (9) - ETAMAX * ETASYS * UF
591 RES (27) = ZA (10) - STCR
592 RES (28) = ZA (11) - E_nernst
593 RES (29) = ZA (12) - V_act
594 RES (30) = ZA (13) - V_ohm
595 RES (31) = ZA (14) - V_conc
596 RES (32) = ZA (15) - V_cell
597 RES (33) = ZA (16) - GMAX
598 RES (34) = ZA (17) - G_standard
599 RES (35) = ZA (18) - G_real
600 RES (36) = ZA (19) - p_H2eq
601 RES (37) = ZA (20) - R_e
602 RES (38) = ZA (21) - i_load
603 RES (39) = ZA (22) - eta_DCAC
604
605
606 IF (FKOMP.EQ.5) GOTO 500
607 GOTO 9999
608 C-----

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609 C   Solution check
610 C-----
611     500 CONTINUE
612         IF (MDOT(1).LT.-1D-10) GOTO 550
613         IF (MDOT(2).LT.-1D-10) GOTO 550
614         IF (MDOT(3).GT.1D-10) GOTO 550
615         IF (MDOT(4).GT.1D-10) GOTO 550
616 C         DO I=1,ANTST
617 C             PRINT*,X_J(MEDIE(3),I),X_J(MEDIE(4),I)
618 C         ENDDO
619         GOTO 9999
620     550 FBETI = .FALSE.
621         GOTO 9999
622 C-----
623 C   Write component information
624 C-----
625     600 CONTINUE
626     KOMDSC = 'Solid oxide fuel cell with given hydrogen utilization'//
627     $      ' and current density. Composition of the depleted fuel'//
628     $      ' is calculated by chemical equilibrium.'//
629     $      ' The voltage efficiency ( $\eta_v$ ) is predicted by an'//
630     $      ' electrochemical model based on the operating conditions.'//
631     $      ' A DC to AC conversion efficiency is also applied.'
632     K_PAR(1) = 'Hydrogen utilization:  $\alpha$  [--]'
633     K_PAR(2) = 'Operating temperature:  $T_{cell}$  [degC]'
634     K_PAR(3) = 'Pressure loss fuel:  $\Delta p_{13}$  [--]'
635     K_PAR(4) = 'Pressure loss air:  $\Delta p_{24}$  [--]'
636     K_PAR(5) = 'Temperature difference between anode and '//
637     $      'cathode outlet:  $\Delta T_{out}$  [degC]'
638     K_PAR(6) = 'Current density:  $i_{load}$  [mA cm-2]'
639     K_PAR(7) = 'DC to AC conversion efficiency:  $\eta_{DCAC}$  [--]'
640     K_LIG(1) = 'Pressure loss fuel:  $p_3=p_1(1-\beta_{13})$ '
641     K_LIG(2) = 'Pressure loss air:  $p_4=p_2(1-\beta_{24})$ '
642     K_LIG(3) = 'Temperature of outlet fuel:  $T_3=T_{cell}$ '
643     K_LIG(4) = 'Temperature of outlet air:  $T_4=T_3-\Delta T_{out}$ '
644     K_LIG(5) = 'Mass flow of used air: '//
645     $      ' $\dot{m}_4=\dot{m}_2$ '//
646     $      ' $\dot{n}_{O_2,actual}M_{O_2}$ '
647     K_LIG(6) = 'Oxygen balance on air side: '//
648     $      ' $\frac{\dot{m}_4}{M_4}y_{O_2,4}=\frac{\dot{m}_2}{M_2}y_{O_2,2}$ '//
649     $      ' $\frac{\dot{m}_2}{M_2}y_{O_2,2}$ '//
650     $      ' $\dot{n}_{O_2,actual}$ '
651     K_LIG(7) = 'Nitrogen balance on air side: '//
652     $      ' $\frac{\dot{m}_4}{M_4}y_{N_2,4}=\frac{\dot{m}_2}{M_2}y_{N_2,2}$ '//
653     $      ' $\frac{\dot{m}_2}{M_2}y_{N_2,2}$ '
654     K_LIG(8) = 'Carbon dioxide balance on air side: '//
655     $      ' $\frac{\dot{m}_4}{M_4}y_{CO_2,4}=\frac{\dot{m}_2}{M_2}y_{CO_2,2}$ '//
656     $      ' $\frac{\dot{m}_2}{M_2}y_{CO_2,2}$ '
657     K_LIG(9) = 'Water balance on air side: '//
658     $      ' $\frac{\dot{m}_4}{M_4}y_{H_2O,4}=\frac{\dot{m}_2}{M_2}y_{H_2O,2}$ '//
659     $      ' $\frac{\dot{m}_2}{M_2}y_{H_2O,2}$ '
660     K_LIG(10) = 'Summation of molar fractions of used air: '//
661     $      ' $y_{O_2,4}+y_{N_2,4}+y_{CO_2,4}+y_{H_2O,4}=1$ '//
662     $      ' $y_{Ar,4}=1$ '
663     K_LIG(11) = 'Partial derivative of Gibbs energy of outlet '//
664     $      'gas with respect to Hydrogen content of gas: '//
665     $      ' $\frac{\partial F}{\partial y_{H_2,out}}$ '//
666     $      ' $\frac{\partial F}{\partial y_{H_2,out}} = \frac{g_{H_2,out}^0}{RT} + \ln(y_{H_2,out} p_3)$ '//
667     $      ' $\sum_j \mu_j \mathbf{A}_j$ '//
668     $      'where  $\mathbf{A}$  is a matrix with information on the'//
669     $      'moles of  $j$  in each mole  $H_2$ . '
670     K_LIG(12) = 'Partial derivative of Gibbs energy of outlet '//
671     $      'gas with respect to Carbon Monoxide content of gas: '//
672     $      ' $\frac{\partial F}{\partial y_{CO,out}}$ '//
673     $      ' $\frac{\partial F}{\partial y_{CO,out}} = \frac{g_{CO,out}^0}{RT} + \ln(y_{CO,out} p_3)$ '//
674     $      ' $\sum_j \mu_j \mathbf{A}_j$ '//
675     $      'where  $\mathbf{A}$  is a matrix with information on the'//
676     $      'moles of  $j$  in each mole  $CO$ . '
677     K_LIG(13) = 'Partial derivative of Gibbs energy of outlet '//

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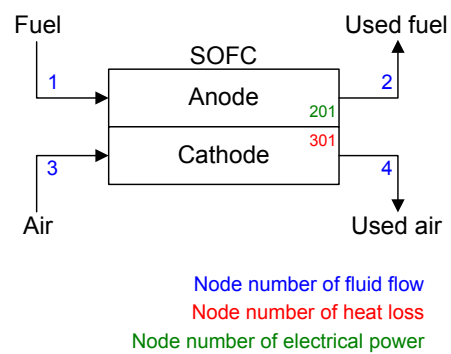
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685 $ 'gas with respect to Carbon Dioxide content of gas:'//
686 $ '$$\frac{\partial F}{\partial n_{\mathrm{CO}_2,\mathrm{out}}}}=$$//
687 $ '\frac{g_{\mathrm{CO}_2,\mathrm{out}}^0}{RT}+'//
688 $ '\ln(y_{\mathrm{CO}_2,\mathrm{out}}p_3)+'//
689 $ '\sum_{j\mathrm{ in H,C,O}}'//
690 $ '\mu_j \mathbf{A}_{\mathrm{CO}_2,j}$$, '//
691 $ 'where $\mathbf{A}$ is a matrix with information on the'//
692 $ ' moles of $j$ in each mole $\mathrm{CO}_2$.$\square$'
693 K_LIG(14) = 'Partial derivative of Gibbs energy of outlet '//
694 $ 'gas with respect to water content of gas:'//
695 $ '$$\frac{\partial F}{\partial n_{\mathrm{H}_2\mathrm{O},\mathrm{out}}}}=$$//
696 $ '\frac{g_{\mathrm{H}_2\mathrm{O},\mathrm{out}}^0}{RT}+'//
697 $ '\ln(y_{\mathrm{H}_2\mathrm{O},\mathrm{out}}p_3)+'//
698 $ '\sum_{j\mathrm{ in H,C,O}}'//
699 $ '\mu_j \mathbf{A}_{\mathrm{H}_2\mathrm{O},j}$$, '//
700 $ 'where $\mathbf{A}$ is a matrix with information on the'//
701 $ ' moles of $j$ in each mole $\mathrm{H}_2\mathrm{O}$.$\square$'
702 K_LIG(15) = 'Partial derivative of Gibbs energy of outlet '//
703 $ 'gas with respect to methane content of gas:'//
704 $ '$$\frac{\partial F}{\partial n_{\mathrm{CH}_4,\mathrm{out}}}}=$$//
705 $ '\frac{g_{\mathrm{CH}_4,\mathrm{out}}^0}{RT}+'//
706 $ '\ln(y_{\mathrm{CH}_4,\mathrm{out}}p_3)+'//
707 $ '\sum_{j\mathrm{ in H,C,O}}'//
708 $ '\mu_j \mathbf{A}_{\mathrm{CH}_4,j}$$, '//
709 $ 'where $\mathbf{A}$ is a matrix with information on the'//
710 $ ' moles of $j$ in each mole $\mathrm{CH}_4$.$\square$'
711 K_LIG(16) = 'Partial derivative of Gibbs energy of outlet '//
712 $ 'gas with respect to nitrogen content of gas:'//
713 $ '$$\frac{\partial F}{\partial n_{\mathrm{N}_2,\mathrm{out}}}}=$$//
714 $ '\frac{g_{\mathrm{N}_2,\mathrm{out}}^0}{RT}+'//
715 $ '\ln(y_{\mathrm{N}_2,\mathrm{out}}p_3)+'//
716 $ '\sum_{j\mathrm{ in H,C,O}}'//
717 $ '\mu_j \mathbf{A}_{\mathrm{N}_2,j}$$, '//
718 $ 'where $\mathbf{A}$ is a matrix with information on the'//
719 $ ' moles of $j$ in each mole $\mathrm{N}_2$.$\square$'
720 K_LIG(17) = 'Molar balance for Hydrogen: '//
721 $ '$\sum_{i\mathrm{ in inlet gas}}'//
722 $ '\dot{n}_{i,\mathrm{in}}\mathbf{A}_{i,\mathrm{H}}-'//
723 $ '\sum_{i\mathrm{ in outlet gas}}'//
724 $ '\dot{n}_{i,\mathrm{out}}\mathbf{A}_{i,\mathrm{H}}$ $\square$'
725 K_LIG(18) = 'Molar balance for Carbon: '//
726 $ '$\sum_{i\mathrm{ in inlet gas}}'//
727 $ '\dot{n}_{i,\mathrm{in}}\mathbf{A}_{i,\mathrm{C}}-'//
728 $ '\sum_{i\mathrm{ in outlet gas}}'//
729 $ '\dot{n}_{i,\mathrm{out}}\mathbf{A}_{i,\mathrm{C}}$ $\square$'
730 K_LIG(19) = 'Molar balance for Nitrogen: '//
731 $ '$\sum_{i\mathrm{ in inlet gas}}'//
732 $ '\dot{n}_{i,\mathrm{in}}\mathbf{A}_{i,\mathrm{N}}-'//
733 $ '\sum_{i\mathrm{ in outlet gas}}'//
734 $ '\dot{n}_{i,\mathrm{out}}\mathbf{A}_{i,\mathrm{N}}$ $\square$'
735 K_LIG(20) = 'Sum of molar fractions in used fuel: '//
736 $ '$\sum_{i\mathrm{ in outlet gas}}=1$ $\square$'
737 K_LIG(21) = 'Gibbs energy of depleted fuel:'//
738 $ '$G = \sum_{i\mathrm{ in outlet gas}}'//
739 $ '\dot{n}_i \left( g_i^0 + R T \ln(y_{ip}) \right) $ $\square$'
740 K_LIG(22) = 'Voltage efficiency from an electrochemical model: '//
741 $ '$\eta_v(T_{\mathrm{cell}},p,y_{i},\alpha_{i,\mathrm{load}})$ $\square$'
742 K_LIG(23) = 'Power production: '//
743 $ '$\dot{E}=\eta_{\max}\eta_v\alpha\eta_{\mathrm{DCAC}}$ '//
744 $ '$\sum_{i\mathrm{ in fuel}} H_{u,i}$, where '//
745 $ '$\alpha=\frac{\dot{n}_{\mathrm{H}_2,\mathrm{cons}}}{\dot{n}_{\mathrm{H}_2}+\dot{n}_{\mathrm{CO}}}$ '//
746 $ '$+4\dot{n}_{\mathrm{CH}_4}$ $ $\square$'
747 K_BET = '$\dot{m}_1 \ge 0$ $\dot{m}_2 \ge 0$ $\dot{m}_3 \ge 0$ $\dot{m}_4 \ge 0$ $ $\square$'
748 $ '$\dot{m}_3 \ge 0$ $\dot{m}_4 \ge 0$ $ $\square$'
749 KMEDDS(1) = 'Fuel inlet $\square$'
750 KMEDDS(2) = 'Air inlet $\square$'
751 KMEDDS(3) = 'Depleted fuel out $\square$'
752 KMEDDS(4) = 'Used air out $\square$'
753 KMEDDS(5) = 'Power $\square$'
754 KMEDDS(6) = 'Heat loss $\square$'
755 K_INP='STRUC sofc sofceq0d_CBM 1 2 3 4 201 301 0.85 800 0 0 0 '//

```

```
761      $      '300 0.95\\\\\\\\'//
762      $      'FLUID fuel H2 0.8 CO2 0.1 N2 0.1\\\\\\\\'//
763      $      'MEDIA 1 fuel 2 SIMPLE_AIR 3 USED_FUEL 4 FLUEGAS\\\\\\\\'//
764      $      'START Y_J USED_FUEL H2 0.2 Y_J USED_FUEL CH4 1e-6\\\\\\\\'//
765      $      'START Y_J USED_FUEL H2O-G 0.3\\\\\\\\'//
766      $      'START Y_J USED_FUEL CO 0.2 Y_J USED_FUEL CO2 0.2 '//
767      $      'Y_J USED_FUEL N2 0.1\\\\\\\\'//
768      $      'START Y_J FLUEGAS N2 0.8 Y_J FLUEGAS O2 0.2\\\\\\\\'//
769      $      'ADDCO m sofc 1 1 t sofc 1 700 p 1 3 '//
770      $      't sofc 2 700 p 2 3\\\\\\\\'//
771      $      'START t sofc 3 800 t sofc 4 800 m sofc 2 100 '//
772      $      'm sofc 3 -10\\\\\\\\'//
773      $      'START p 2 3 p 3 3 p 4 3 \\\\\\\'//
774      $      'ADDCO q sofc 301 0'
775      GOTO 9999
776  C
777  9999 CONTINUE
778      RETURN
779      END
780
781  C=====
end
```

Flow sheet of SOFC component test with node numbers



DNA Input for SOFC component test

1/2

```
1 title SOFC component test
2
3 fluid FUEL H2 0.2614 N2 0.30198 CO 0.1814 CO2 0.1179 H2O-G 0.1269 CH4 0.01042
4
5 media 3 STANDARD_AIR 1 FUEL 2 USED_FUEL 4 USED_AIR
6
7 C -----SOFC-----
8 struc sofc sofceq0d_CBM /
9 {fuel and air inlets} 1 3 /
10 {fuel and air outlets} 2 4 /
11 {nodes for power and heat loss} 201 301 /
12 {parameters: utilization, temperature} 0.85 800 /
13 {pressure loss ratios} 0 0 /
14 {temperature difference between anode and cathode outlet} 0 /
15 {current density [mA/cm2]} 300 /
16 {DC to AC conversion efficiency [-]} 1
17
18 addco p 3 1 t sofc 3 600
19 addco p 1 1 t sofc 1 650
20 addco e sofc 201 -10000
21 addco q sofc 301 0
22
23
24
25
26 C ~~~~~
27 C ~~~ Start of list of generated initial guesses.
28 C ~~~ The values are the results of the latest simulation.
29 C ~~~~~
30 START M sofc 1 0.3570149203519879E+01 {~~}
31 START P sofc 1 0.1000000000000002E+01 {~~}
32 START H sofc 1 -0.3556798254615437E+04 {~~}
33 START M sofc 3 0.2821245195002270E+02 {~~}
34 START P sofc 3 0.1000000000000002E+01 {~~}
35 START H sofc 3 0.5194065598541852E+03 {~~}
36 START M sofc 2 -0.4653675564564562E+01 {~~}
37 START P sofc 2 0.1000000000000002E+01 {~~}
38 START H sofc 2 -0.6077944726815711E+04 {~~}
39 START M sofc 4 -0.2712892558897801E+02 {~~}
40 START P sofc 4 0.1000000000000002E+01 {~~}
41 START H sofc 4 0.7460750684058085E+03 {~~}
42 START E sofc 201 -0.1000000000000002E+05 {~~}
43 START Q sofc 301 0.0000000000000000E+00 {~~}
44 START ZA sofc 1 0.9305205152080904E+05 {~~}
45 START ZA sofc 2 0.8334089162545065E+05 {~~}
46 START ZA sofc 3 0.1171736976840727E+06 {~~}
47 START ZA sofc 4 0.2887364309244900E+06 {~~}
48 START ZA sofc 5 -0.4395688774684369E+06 {~~}
49 START ZA sofc 6 0.6884847150125958E+00 {~~}
50 START ZA sofc 7 0.8454116292315869E+00 {~~}
51 START ZA sofc 8 0.8500000000000016E+00 {~~}
52 START ZA sofc 9 0.4947450369268662E+00 {~~}
53 START ZA sofc 10 0.4097249128244875E+00 {~~}
54 START ZA sofc 11 0.9452308098598988E+00 {~~}
55 START ZA sofc 12 0.1082124265828745E+00 {~~}
56 START ZA sofc 13 0.7147434745365793E-02 {~~}
57 START ZA sofc 14 0.3076182956811065E-01 {~~}
58 START ZA sofc 15 0.7991091189635479E+00 {~~}
59 START ZA sofc 16 -0.8462030083349127E+05 {~~}
60 START ZA sofc 17 -0.1885369880714485E+06 {~~}
61 START ZA sofc 18 -0.1824011893786647E+06 {~~}
62 START ZA sofc 19 0.2778328680585008E+00 {~~}
63 START ZA sofc 20 0.2335762988681631E-01 {~~}
64 START ZA sofc 21 0.4356137835365532E+05 {~~}
65 START ZA sofc 22 0.3000000000000006E+03 {~~}
66 START Y_J USED_FUEL H2 0.4175231528646270E-01 {~~}
67 START Y_J USED_FUEL CO 0.2943327774588393E-01 {~~}
68 START Y_J USED_FUEL CO2 0.2739639104926799E+00 {~~}
69 START Y_J USED_FUEL H2O-G 0.3590352285377990E+00 {~~}
70 START Y_J USED_FUEL CH4 0.3577116348414438E-07 {~~}
71 START Y_J USED_FUEL N2 0.2958152321660127E+00 {~~}
72 START Y_J USED_AIR O2 0.1790704565457096E+00 {~~}
73 START Y_J USED_AIR N2 0.8006264279316373E+00 {~~}
74 START Y_J USED_AIR CO2 0.3107619722855365E-03 {~~}
```

DNA Input for SOFC component test

2/2

```
75 START Y_J  USED AIR      H2O-G      0.1046231973361306E-01 {~~}
76 START Y_J  USED AIR      AR          0.9530033816756465E-02 {~~}
77 C ~~~~~
    ~~~~~
78 C ~~ End of generated initial guesses.
79 C ~~~~~
    ~~~~~
end
```

DNA Output for SOFC component test

1/2

```
1  SOFC component test
2  RUN NUMBER      1
3
4
5
6  ALGEBRAIC VARIABLES
7  NO |      TO      | MEDIA      |      M      |      T      |      P      |      H      | ENERGY | X |      S      |      V      |      U      |
8  DE | COMPONENT |          | [kg/s] | [C] | [bar] | [kJ/kg] | [kJ/s] | | [kJ/kg K] | [m3/kg] | [kJ/kg] |
9  -----
10  1 |sofc      | FUEL      |      3.57 | 650.00 | 1.000 | -3556.8 | 2.021E+04 | - | 10.5509 | 3.5354 | -3910.3 |
11  3 |sofc      | STANDARD_AIR |      28.21 | 600.00 | 1.000 | 519.4 | | | 8.0291 | 2.5159 | 267.8 |
12  2 |sofc      | USED_FUEL  |      -4.65 | 800.00 | 1.000 | -6077.9 | | | 9.1127 | 3.2186 | -6399.8 |
13  4 |sofc      | USED_AIR   |     -27.13 | 800.00 | 1.000 | 746.1 | | | 8.2703 | 3.1043 | 435.6 |
14 201 |sofc      | ELECT_POWER |          |          |          |          | -1.000E+04 | |          |          |          |
15 301 |sofc      | HEAT       |          |          |          |          | 0.000E+00 | |          |          |          |
16  -----
17
18  ELEC. POWER PRODUCTION = 10000.0000 kW
19  NET POWER PRODUCTION  = 10000.0000 kW
20  FUEL CONSUMPTION (LHV) = 20212.4312 kJ/s
21  FUEL CONSUMPTION (HHV) = 41892.1896 kJ/s
22  THERMAL EFFICIENCY (LHV) = 0.4947
23  THERMAL EFFICIENCY (HHV) = 0.2387
24
25  MAXIMUM RELATIVE ERROR = 2.1736E-14
26  COMPUTER ACCURACY      = 1.0842E-19
27
28
29
30  IDEAL GAS COMPOSITION (MOLAR BASE):
31
32          | FUEL      | STANDARD_AIR | USED_FUEL  | USED_AIR   |
33  -----
34  HYDROGEN      | 0.2614E+00 | 0.0000E+00 | 0.4175E-01 | 0.0000E+00 |
35  OXYGEN        | 0.0000E+00 | 0.2075E+00 | 0.0000E+00 | 0.1791E+00 |
36  NITROGEN      | 0.3020E+00 | 0.7729E+00 | 0.2958E+00 | 0.8006E+00 |
37  CARBON MONOXIDE | 0.1814E+00 | 0.0000E+00 | 0.2943E-01 | 0.0000E+00 |
38  CARBON DIOXIDE | 0.1179E+00 | 0.3000E-03 | 0.2740E+00 | 0.3108E-03 |
39  WATER (I.G.)  | 0.1269E+00 | 0.1010E-01 | 0.3590E+00 | 0.1046E-01 |
40  METHANE       | 0.1042E-01 | 0.0000E+00 | 0.3577E-07 | 0.0000E+00 |
41  ARGON         | 0.0000E+00 | 0.9200E-02 | 0.0000E+00 | 0.9530E-02 |
42  -----
43  MEAN MOLE MASS | 0.2171E+02 | 0.2885E+02 | 0.2772E+02 | 0.2874E+02 |
44  NET CALORI VALUE | 0.5662E+04 | 0.0000E+00 | 0.6647E+03 | 0.0000E+00 |
45  GRS CALORI VALUE | 0.1173E+05 | 0.0000E+00 | 0.2453E+04 | 0.0000E+00 |
46  -----
47
48  MEDIUM 200 : ELECTRICAL POWER
49  MEDIUM 300 : HEAT
50  MEDIUM 301 : PRODUCT HEAT
51
52
53  NUMBER OF CLOSED INTERNAL LOOPS IN THE SYSTEM: 0
54
```


DNA Output for SOFC component test

2/2

```
54
55
56
57
58 SOLUTION FOR THE INDEPENDENT ALGEBRAIC VARIABLES :
59
60
61 VARIABLE NO | COMPONENT | NAME | VALUE |
62 -----
63 1 | sofc | MULTIPLIER H | 0.9305E+05 |
64 2 | sofc | MULTIPLIER C | 0.8334E+05 |
65 3 | sofc | MULTIPLIER N | 0.1172E+06 |
66 4 | sofc | MULTIPLIER O | 0.2887E+06 |
67 5 | sofc | GIBBS ENERGY | -.4396E+06 |
68 6 | sofc | ETAMAX | 0.6885E+00 |
69 7 | sofc | ETASYS | 0.8454E+00 |
70 8 | sofc | UF | 0.8500E+00 |
71 9 | sofc | ETATOT | 0.4947E+00 |
72 10 | sofc | STCR | 0.4097E+00 |
73 11 | sofc | E_nernst | 0.9452E+00 |
74 12 | sofc | V_act | 0.1082E+00 |
75 13 | sofc | V_ohm | 0.7147E-02 |
76 14 | sofc | V_conc | 0.3076E-01 |
77 15 | sofc | V_cell | 0.7991E+00 |
78 16 | sofc | GMAX | -.8462E+05 |
79 17 | sofc | G(T) | -.1885E+06 |
80 18 | sofc | G(p,T) | -.1824E+06 |
81 19 | sofc | p_H2eq | 0.2778E+00 |
82 20 | sofc | R_e | 0.2336E-01 |
83 21 | sofc | Area [cm^2] | 0.4356E+05 |
84 22 | sofc | i_load | 0.3000E+03 |
85 23 | sofc | eta_DCAC | 0.1000E+01 |
86 -----
87
88 =====
89 #####
end
```

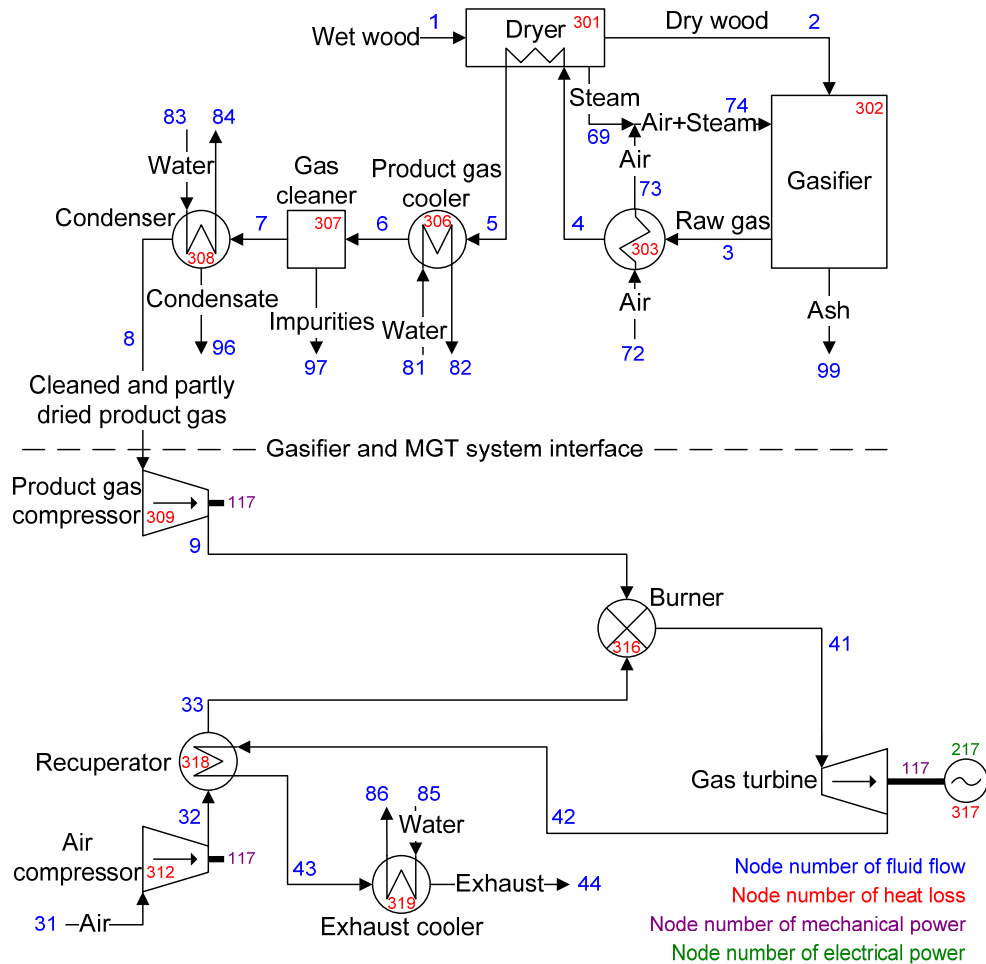
Appendix C MGT PLANT MODEL LISTING

Included in this Appendix are:

- Flow sheet of MGT scenario with node numbers (1 page)
- DNA Input for MGT scenario (9 pages)
- DNA Output for MGT scenario (6 pages)

The input and output data only represent one simulation using the reference conditions.

Flow sheet of MGT scenario with node numbers



DNA Input for MGT scenario

1/9

```
1 title Biomass gasification (Viking) + MGT incl. recuperation
2 C Wood is dried and gasified. The gasification is atmospheric,
3 C based on air, and almost reaches equilibrium. The produced
4 C product gas (PG) composition and the cold gas efficiency is
5 C similar to that from the Viking gasifier.
6 C Power and heat production by a MGT system.
7
8
9 C #####
10 C #####
11 C #####
12 C -----GASIFIER PART-----
13 C #####
14 C #####
15 C #####
16
17 C ##Media##
18 media 1 Wood 2 DryWood
19 media 73 STANDARD_AIR 3 raw_PG 99 Ash
20
21 C ##Fuel composition##
22 solid Wood C 0.488 H .062 O .439 S .0002 N 0.0017 ASH .0091
23 + LHV 18280 CP 1.35 MOI .322
24 C [Ahrenfeldt, J. et al., Energy & Fuels 2006, 20, 2672-2680] without Cl.
25
26
27
28 C #####
29 C -----DRYER-----
30 C #####
31 struc Dryer DRYER_03 1 64 2 61 301 0.05 0.005
32
33 C Fuel input (plant size):
34 addco m Dryer 1 0.043
35
36 addco t Dryer 1 15 p 1 1.013
37 addco p 2 1.008 t Dryer 2 150
38 addco q Dryer 301 0
39
40
41
42 C #####
43 C -----GASIFIER-----
44 C #####
45 struc Gasifier GASIFI_3 8 2 26 74 3 99 302 1 3 4 6 7 9 11 36 /
46 0.998 800 0.005 0 1.0 0.01
47 C Variable constitution parameter: Number of calculated gas components 8
48 C Nodes: Inlet fuel 2; inlet water 26; inlet air 74; outlet PG 3,
49 C outlet ash 99, heat loss 302
50 C Integer Parameters: Calculated gas compounds H2 (1), N2 (3), CO (4),
51 C CO2 (6), H2O (7), H2S (9), CH4 (11), Ar (36)
52 C Real parameter: Pressure 1 bar, Eq. temperature 800 degC, Pressure loss 0,
53 C Water-to-fuel ratio 0, carbon conversion factor 1,
54 C non-equilibrium methane 0.01.
55
56 addco t Gasifier 3 800
57 addco t Gasifier 26 150
58 addco p 99 1.013
59 addco q Gasifier 302 0
60
61
62
63 C #####
64 C -----GASIFIER AIR PREHEATER-----
65 C #####
66 struc airpreheat heatex_2 3 4 72 73 303 20 0.005 0.005
67 addco t airpreheat 72 15
68 addco q airpreheat 303 0
69
70
71
72 C #####
73 C -----STEAM HEATER-----
74 C #####
75 struc steamheater heatex_1 4 5 63 64 304 0.005 0.005
76
```

DNA Input for MGT scenario

2/9

```
77 media 63 STEAM-HF
78
79 addco t steamheater 64 250
80 addco q steamheater 304 0
81
82
83
84 C #####
85 C -----STEAM BLOWER-----
86 C #####
87 struc steamblower COMPRE_1 61 62 305 105 0.6 0.98
88
89
90
91 C #####
92 C -----SPLITTER-----
93 C #####
94 struc split1 SPLITTER 62 63 69
95
96
97
98 C #####
99 C -----MIXER-----
100 C #####
101 struc mix1 MIXER_02 73 69 74
102
103 media 74 humid_air
104
105
106
107 C #####
108 C -----GAS COOLER-----
109 C #####
110 struc gascooler GASCOOL1 5 6 98 81 82 306 0.005 0.005
111
112 media 81 STEAM-HF 6 cold_PG
113
114 addco t gascooler 6 90
115 addco t gascooler 81 30 p 81 1.013
116 addco t gascooler 82 80
117 addco q gascooler 306 0
118
119
120
121 C #####
122 C -----GAS CLEANING-----
123 C #####
124 struc gasclean GASCLE_1 6 7 97 307 0.0049
125 C Pressure loss is taken from paper about Viking
126
127 media 7 clean_PG 97 impurities
128
129 addco q gasclean 307 0
130
131
132
133 C #####
134 C -----CONDENSER-----
135 C #####
136 struc condenser GASCOOL1 7 8 96 83 84 308 0.005 0.005
137
138 media 83 STEAM-HF 8 dry_PG
139
140 addco t condenser 8 50
141 addco t condenser 83 30 p 83 1.013
142 addco t condenser 84 80
143 addco q condenser 308 0
144
145
146
147 C #####
148 C #####
149 C #####
150 C -----MGT PART-----
151 C #####
152 C #####
```

DNA Input for MGT scenario

3/9

```
153 C #####
154
155
156
157 C #####
158 C -----PG COMPRESSOR-----
159 C #####
160 struc PGcompressor compre_1 8 9 309 117 0.75 0.98
161 C Isentropic efficiency from L. Fryda et al. (2008)
162
163
164
165 C #####
166 C -----AIR COMPRESSOR-----
167 C #####
168 struc aircompressor compre_1 31 32 312 117 0.75 0.98
169 C Isentropic efficiency from L. Fryda et al. (2008)
170
171 media 31 STANDARD_AIR
172
173 addco p 31 1.013 t aircompressor 31 15
174
175
176
177 C #####
178 C -----RECUPERATOR-----
179 C #####
180 struc recuperator heatex_4 42 43 32 33 318 0.85 0.01 0.01
181 addco q recuperator 318 0
182
183
184
185 C #####
186 C -----BURNER-----
187 C #####
188 struc burner GASBUR_3 33 9 41 316 0.999374
189
190 media 41 FLUE_GAS
191
192 addco q burner 316 0
193
194 C BURNER OPERATING PRESSURE:
195 addco p 9 3.75
196
197
198
199 C #####
200 C -----GAS TURBINE-----
201 C #####
202 struc GT turbin_1 41 42 117 0.84
203 C Isentropic efficiency from L. Fryda et al. (2008)
204
205 addco t GT 41 900
206
207
208
209 C #####
210 C -----GENERATOR-----
211 C #####
212 struc generator sim_gene 217 317 117 0.95
213
214
215
216 C #####
217 C -----DISTRICT HEATING-----
218 C #####
219 struc exhaustcooler heatex_2 43 44 85 86 319 90 0.010 0.005
220
221 media 85 STEAM-HF
222
223 addco p 44 1.013
224 addco p 85 1.013 t exhaustcooler 85 30
225 addco t exhaustcooler 86 80
226 addco q exhaustcooler 319 0
227
228
```

```

229
230 C Reference conditions for exergy
231 xergy p 1 t 15
232
233
234
235
236 C ~~~~~
~~~~~
237 C ~~ Start of list of generated initial guesses.
238 C ~~ The values are the results of the latest simulation.
239 C ~~~~~
~~~~~
240 START M      Dryer          1  0.43000000000000009E-01 {~~}
241 START P      1  0.10130000000000002E+01 {~~}
242 START H      Dryer          1  -0.8621618755529553E+04 {~~}
243 START M      Dryer          64  0.2000459030657094E+00 {~~}
244 START P      64  0.998000000000000021E+00 {~~}
245 START H      Dryer          64  -0.1299653551379775E+05 {~~}
246 START M      Dryer          2  -0.3068842105263164E-01 {~~}
247 START P      2  0.10080000000000002E+01 {~~}
248 START H      Dryer          2  -0.5497059220211011E+04 {~~}
249 START M      Dryer          61  -0.2123574820130778E+00 {~~}
250 START P      61  0.993000000000000021E+00 {~~}
251 START H      Dryer          61  -0.1319443607829822E+05 {~~}
252 START Q      Dryer          301 0.0000000000000000E+00 {~~}
253 START X_J    DryWood        H2  0.589000000000000011E-01 {~~}
254 START X_J    DryWood        O2  0.417050000000000009E+00 {~~}
255 START X_J    DryWood        N2  0.161500000000000003E-02 {~~}
256 START X_J    DryWood        CO  0.0000000000000000E+00 {~~}
257 START X_J    DryWood        NO  0.0000000000000000E+00 {~~}
258 START X_J    DryWood        CO2 0.0000000000000000E+00 {~~}
259 START X_J    DryWood        H2O-L 0.50000000000000009E-01 {~~}
260 START X_J    DryWood        NH3 0.0000000000000000E+00 {~~}
261 START X_J    DryWood        H2S 0.0000000000000000E+00 {~~}
262 START X_J    DryWood        SO2 0.0000000000000000E+00 {~~}
263 START X_J    DryWood        CH4 0.0000000000000000E+00 {~~}
264 START X_J    DryWood        C2H6 0.0000000000000000E+00 {~~}
265 START X_J    DryWood        C3H8 0.0000000000000000E+00 {~~}
266 START X_J    DryWood        C4H10-N 0.0000000000000000E+00 {~~}
267 START X_J    DryWood        C4H10-I 0.0000000000000000E+00 {~~}
268 START X_J    DryWood        C5H12 0.0000000000000000E+00 {~~}
269 START X_J    DryWood        C6H14 0.0000000000000000E+00 {~~}
270 START X_J    DryWood        C7H16 0.0000000000000000E+00 {~~}
271 START X_J    DryWood        C8H18 0.0000000000000000E+00 {~~}
272 START X_J    DryWood        C2H4 0.0000000000000000E+00 {~~}
273 START X_J    DryWood        C3H6 0.0000000000000000E+00 {~~}
274 START X_J    DryWood        C5H10 0.0000000000000000E+00 {~~}
275 START X_J    DryWood        C6H12-1 0.0000000000000000E+00 {~~}
276 START X_J    DryWood        C7H14 0.0000000000000000E+00 {~~}
277 START X_J    DryWood        C2H2 0.0000000000000000E+00 {~~}
278 START X_J    DryWood        C6H6 0.0000000000000000E+00 {~~}
279 START X_J    DryWood        C6H12-C 0.0000000000000000E+00 {~~}
280 START X_J    DryWood        C 0.46360000000000009E+00 {~~}
281 START X_J    DryWood        S 0.19000000000000004E-03 {~~}
282 START X_J    DryWood        NO2 0.0000000000000000E+00 {~~}
283 START X_J    DryWood        HCN 0.0000000000000000E+00 {~~}
284 START X_J    DryWood        COS 0.0000000000000000E+00 {~~}
285 START X_J    DryWood        N2O 0.0000000000000000E+00 {~~}
286 START X_J    DryWood        NO3 0.0000000000000000E+00 {~~}
287 START X_J    DryWood        SO3 0.0000000000000000E+00 {~~}
288 START X_J    DryWood        AR 0.0000000000000000E+00 {~~}
289 START X_J    DryWood        ASH 0.864500000000000019E-02 {~~}
290 START X_J    DryWood        TAR 0.0000000000000000E+00 {~~}
291 START M      Gasifier        2  0.3068842105263164E-01 {~~}
292 START H      Gasifier        2  -0.5497059220211011E+04 {~~}
293 START M      Gasifier        26 0.0000000000000000E+00 {~~}
294 START P      26 0.10030000000000002E+01 {~~}
295 START H      Gasifier        26  -0.1319450918722708E+05 {~~}
296 START M      Gasifier        74  0.5485206982616304E-01 {~~}
297 START P      74  0.10030000000000002E+01 {~~}
298 START H      Gasifier        74  -0.2398848478333938E+04 {~~}
299 START M      Gasifier        3  -0.8527518947879467E-01 {~~}
300 START P      3  0.998000000000000021E+00 {~~}
301 START H      Gasifier        3  -0.3507877913073770E+04 {~~}
302 START M      Gasifier        99  -0.26530140000000006E-03 {~~}

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303 START P
304 START H Gasifier
305 START Q Gasifier
306 START ZA Gasifier
307 START ZA Gasifier
308 START ZA Gasifier
309 START ZA Gasifier
310 START ZA Gasifier
311 START ZA Gasifier
312 START ZA Gasifier
313 START Y_J raw_PG
314 START Y_J raw_PG
315 START Y_J raw_PG
316 START Y_J raw_PG
317 START Y_J raw_PG
318 START Y_J raw_PG
319 START Y_J raw_PG
320 START Y_J raw_PG
321 START Y_J raw_PG
322 START Y_J raw_PG
323 START Y_J raw_PG
324 START Y_J raw_PG
325 START Y_J raw_PG
326 START Y_J raw_PG
327 START Y_J raw_PG
328 START X_J Ash
329 START X_J Ash
330 START M airpreheat
331 START H airpreheat
332 START M airpreheat
333 START P
334 START H airpreheat
335 START M airpreheat
336 START P
337 START H airpreheat
338 START M airpreheat
339 START P
340 START H airpreheat
341 START Q airpreheat
342 START ZA airpreheat
343 START M steamheater
344 START H steamheater
345 START M steamheater
346 START P
347 START H steamheater
348 START M steamheater
349 START P
350 START H steamheater
351 START M steamheater
352 START H steamheater
353 START Q steamheater
354 START ZA steamheater
355 START M steamblower
356 START H steamblower
357 START M steamblower
358 START P
359 START H steamblower
360 START Q steamblower
361 START W steamblower
362 START M split1
363 START H split1
364 START M split1
365 START H split1
366 START M split1
367 START P
368 START H split1
369 START M mix1
370 START H mix1
371 START M mix1
372 START H mix1
373 START M mix1
374 START H mix1
375 START Y_J humid_air
376 START Y_J humid_air
377 START Y_J humid_air
378 START Y_J humid_air

99 0.10130000000000002E+01 {~~}
99 -0.43080000000000008E+04 {~~}
302 0.0000000000000000E+00 {~~}
1 0.8500945239865259E+05 {~~}
2 0.4363965291425181E+05 {~~}
3 0.1172765217993688E+06 {~~}
4 0.3124902840469579E+06 {~~}
5 0.1827651987487792E+06 {~~}
6 0.2292482774424775E+06 {~~}
7 -0.3279719879436739E+06 {~~}
H2 0.2538114658675978E+00 {~~}
O2 0.0000000000000000E+00 {~~}
N2 0.2896541868376543E+00 {~~}
CO 0.1761818347160900E+00 {~~}
NO 0.0000000000000000E+00 {~~}
CO2 0.1144395150133745E+00 {~~}
H2O-G 0.1523098114753787E+00 {~~}
NH3 0.0000000000000000E+00 {~~}
H2S 0.4615796164902311E-04 {~~}
SO2 0.0000000000000000E+00 {~~}
CH4 0.1011293223314740E-01 {~~}
NO2 0.0000000000000000E+00 {~~}
HCN 0.0000000000000000E+00 {~~}
COS 0.0000000000000000E+00 {~~}
AR 0.3444095895110056E-02 {~~}
C 0.0000000000000000E+00 {~~}
ASH 0.10000000000000002E+01 {~~}
3 0.8527518947879467E-01 {~~}
3 -0.3507877913073770E+04 {~~}
4 -0.8527518947879467E-01 {~~}
4 0.99300000000000021E+00 {~~}
4 -0.3918630307677503E+04 {~~}
72 0.4254049087879459E-01 {~~}
72 0.10080000000000002E+01 {~~}
72 -0.9883454496688249E+02 {~~}
73 -0.4254049087879459E-01 {~~}
73 0.10030000000000002E+01 {~~}
73 0.7245454291500140E+03 {~~}
303 0.0000000000000000E+00 {~~}
1 0.3502698827870191E+02 {~~}
4 0.8527518947879467E-01 {~~}
4 -0.3918630307677503E+04 {~~}
5 -0.8527518947879467E-01 {~~}
5 0.98800000000000021E+00 {~~}
5 -0.4375257198957321E+04 {~~}
63 0.2000459030657094E+00 {~~}
63 0.10030000000000002E+01 {~~}
63 -0.1319118556200298E+05 {~~}
64 -0.2000459030657094E+00 {~~}
64 -0.1299653551379775E+05 {~~}
304 0.0000000000000000E+00 {~~}
1 0.3893894467499939E+02 {~~}
61 0.2123574820130778E+00 {~~}
61 -0.1319443607829822E+05 {~~}
62 -0.2123574820130778E+00 {~~}
62 0.10030000000000002E+01 {~~}
62 -0.1319118556200298E+05 {~~}
305 -0.1408717256529193E-01 {~~}
105 0.7043586282645935E+00 {~~}
62 0.2123574820130778E+00 {~~}
62 -0.1319118556200298E+05 {~~}
63 -0.2000459030657094E+00 {~~}
63 -0.1319118556200298E+05 {~~}
69 -0.1231157894736844E-01 {~~}
69 0.10030000000000002E+01 {~~}
69 -0.1319118556200298E+05 {~~}
73 0.4254049087879459E-01 {~~}
73 0.7245454291500140E+03 {~~}
69 0.1231157894736844E-01 {~~}
69 -0.1319118556200299E+05 {~~}
74 -0.5485206982616304E-01 {~~}
74 -0.2398848478333938E+04 {~~}
H2 0.0000000000000000E+00 {~~}
O2 0.1417803964772677E+00 {~~}
N2 0.5281063539146036E+00 {~~}
CO 0.0000000000000000E+00 {~~}

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379 START Y_J humid_air NO 0.0000000000000000E+00 {~~}
380 START Y_J humid_air CO2 0.2049837057502667E-03 {~~}
381 START Y_J humid_air H2O-G 0.3236220989260387E+00 {~~}
382 START Y_J humid_air NH3 0.0000000000000000E+00 {~~}
383 START Y_J humid_air H2S 0.0000000000000000E+00 {~~}
384 START Y_J humid_air SO2 0.0000000000000000E+00 {~~}
385 START Y_J humid_air CH4 0.0000000000000000E+00 {~~}
386 START Y_J humid_air C2H6 0.0000000000000000E+00 {~~}
387 START Y_J humid_air C3H8 0.0000000000000000E+00 {~~}
388 START Y_J humid_air C4H10-N 0.0000000000000000E+00 {~~}
389 START Y_J humid_air C4H10-I 0.0000000000000000E+00 {~~}
390 START Y_J humid_air C5H12 0.0000000000000000E+00 {~~}
391 START Y_J humid_air C6H14 0.0000000000000000E+00 {~~}
392 START Y_J humid_air C7H16 0.0000000000000000E+00 {~~}
393 START Y_J humid_air C8H18 0.0000000000000000E+00 {~~}
394 START Y_J humid_air C2H4 0.0000000000000000E+00 {~~}
395 START Y_J humid_air C3H6 0.0000000000000000E+00 {~~}
396 START Y_J humid_air C5H10 0.0000000000000000E+00 {~~}
397 START Y_J humid_air C6H12-1 0.0000000000000000E+00 {~~}
398 START Y_J humid_air C7H14 0.0000000000000000E+00 {~~}
399 START Y_J humid_air C2H2 0.0000000000000000E+00 {~~}
400 START Y_J humid_air C6H6 0.0000000000000000E+00 {~~}
401 START Y_J humid_air C6H12-C 0.0000000000000000E+00 {~~}
402 START Y_J humid_air C 0.0000000000000000E+00 {~~}
403 START Y_J humid_air S 0.0000000000000000E+00 {~~}
404 START Y_J humid_air NO2 0.0000000000000000E+00 {~~}
405 START Y_J humid_air HCN 0.0000000000000000E+00 {~~}
406 START Y_J humid_air COS 0.0000000000000000E+00 {~~}
407 START Y_J humid_air N2O 0.0000000000000000E+00 {~~}
408 START Y_J humid_air NO3 0.0000000000000000E+00 {~~}
409 START Y_J humid_air SO3 0.0000000000000000E+00 {~~}
410 START Y_J humid_air AR 0.6286166976341510E-02 {~~}
411 START Y_J humid_air ASH 0.0000000000000000E+00 {~~}
412 START Y_J humid_air TAR 0.0000000000000000E+00 {~~}
413 START Y_J humid_air CH3OH 0.0000000000000000E+00 {~~}
414 START M gascooler 5 0.8527518947879467E-01 {~~}
415 START H gascooler 5 -0.4375257198957321E+04 {~~}
416 START M gascooler 6 -0.8527518947879467E-01 {~~}
417 START P 6 0.9830000000000002E+00 {~~}
418 START H gascooler 6 -0.4624611248324039E+04 {~~}
419 START M gascooler 98 0.0000000000000000E+00 {~~}
420 START P 98 0.9830000000000002E+00 {~~}
421 START H gascooler 98 -0.1559408877861427E+05 {~~}
422 START M gascooler 81 0.1016636501943091E+00 {~~}
423 START P 81 0.1013000000000002E+01 {~~}
424 START H gascooler 81 -0.1584524528596514E+05 {~~}
425 START M gascooler 82 -0.1016636501943091E+00 {~~}
426 START P 82 0.1008000000000002E+01 {~~}
427 START H gascooler 82 -0.1563608779686839E+05 {~~}
428 START Q gascooler 306 0.0000000000000000E+00 {~~}
429 START Y_J cold_PG H2 0.2538114658675980E+00 {~~}
430 START Y_J cold_PG O2 0.0000000000000000E+00 {~~}
431 START Y_J cold_PG N2 0.2896541868376545E+00 {~~}
432 START Y_J cold_PG CO 0.1761818347160902E+00 {~~}
433 START Y_J cold_PG NO 0.0000000000000000E+00 {~~}
434 START Y_J cold_PG CO2 0.1144395150133747E+00 {~~}
435 START Y_J cold_PG H2O-G 0.1523098114753787E+00 {~~}
436 START Y_J cold_PG NH3 0.0000000000000000E+00 {~~}
437 START Y_J cold_PG H2S 0.4615796164902315E-04 {~~}
438 START Y_J cold_PG SO2 0.0000000000000000E+00 {~~}
439 START Y_J cold_PG CH4 0.1011293223314741E-01 {~~}
440 START Y_J cold_PG C2H6 0.0000000000000000E+00 {~~}
441 START Y_J cold_PG C3H8 0.0000000000000000E+00 {~~}
442 START Y_J cold_PG C4H10-N 0.0000000000000000E+00 {~~}
443 START Y_J cold_PG C4H10-I 0.0000000000000000E+00 {~~}
444 START Y_J cold_PG C5H12 0.0000000000000000E+00 {~~}
445 START Y_J cold_PG C6H14 0.0000000000000000E+00 {~~}
446 START Y_J cold_PG C7H16 0.0000000000000000E+00 {~~}
447 START Y_J cold_PG C8H18 0.0000000000000000E+00 {~~}
448 START Y_J cold_PG C2H4 0.0000000000000000E+00 {~~}
449 START Y_J cold_PG C3H6 0.0000000000000000E+00 {~~}
450 START Y_J cold_PG C5H10 0.0000000000000000E+00 {~~}
451 START Y_J cold_PG C6H12-1 0.0000000000000000E+00 {~~}
452 START Y_J cold_PG C7H14 0.0000000000000000E+00 {~~}
453 START Y_J cold_PG C2H2 0.0000000000000000E+00 {~~}
454 START Y_J cold_PG C6H6 0.0000000000000000E+00 {~~}

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455	START	Y_J	cold_PG	C6H12-C	0.0000000000000000E+00	{~~}
456	START	Y_J	cold_PG	C	0.0000000000000000E+00	{~~}
457	START	Y_J	cold_PG	S	0.0000000000000000E+00	{~~}
458	START	Y_J	cold_PG	NO2	0.0000000000000000E+00	{~~}
459	START	Y_J	cold_PG	HCN	0.0000000000000000E+00	{~~}
460	START	Y_J	cold_PG	COS	0.0000000000000000E+00	{~~}
461	START	Y_J	cold_PG	N2O	0.0000000000000000E+00	{~~}
462	START	Y_J	cold_PG	NO3	0.0000000000000000E+00	{~~}
463	START	Y_J	cold_PG	SO3	0.0000000000000000E+00	{~~}
464	START	Y_J	cold_PG	AR	0.3444095895110058E-02	{~~}
465	START	M	gasclean	6	0.8527518947879467E-01	{~~}
466	START	H	gasclean	6	-0.4624611248324039E+04	{~~}
467	START	M	gasclean	7	-0.8526899202586889E-01	{~~}
468	START	P		7	0.9781000000000021E+00	{~~}
469	START	H	gasclean	7	-0.4624908439609420E+04	{~~}
470	START	M	gasclean	97	-0.6197452925764206E-05	{~~}
471	START	P		97	0.9781000000000021E+00	{~~}
472	START	H	gasclean	97	-0.5356408846834947E+03	{~~}
473	START	Q	gasclean	307	0.0000000000000000E+00	{~~}
474	START	Y_J	clean_PG	H2	0.2538231818282903E+00	{~~}
475	START	Y_J	clean_PG	O2	0.0000000000000000E+00	{~~}
476	START	Y_J	clean_PG	N2	0.2896675573016551E+00	{~~}
477	START	Y_J	clean_PG	CO	0.1761899672858430E+00	{~~}
478	START	Y_J	clean_PG	NO	0.0000000000000000E+00	{~~}
479	START	Y_J	clean_PG	CO2	0.1144447975519509E+00	{~~}
480	START	Y_J	clean_PG	H2O-G	0.1523168421103353E+00	{~~}
481	START	Y_J	clean_PG	CH4	0.1011339904703275E-01	{~~}
482	START	Y_J	clean_PG	NO2	0.0000000000000000E+00	{~~}
483	START	Y_J	clean_PG	AR	0.3444254874894482E-02	{~~}
484	START	Y_J	impurities	H2O-G	0.0000000000000000E+00	{~~}
485	START	Y_J	impurities	NH3	0.0000000000000000E+00	{~~}
486	START	Y_J	impurities	H2S	0.1000000000000002E+01	{~~}
487	START	Y_J	impurities	SO2	0.0000000000000000E+00	{~~}
488	START	Y_J	impurities	HCN	0.0000000000000000E+00	{~~}
489	START	Y_J	impurities	COS	0.0000000000000000E+00	{~~}
490	START	Y_J	impurities	AR	0.0000000000000000E+00	{~~}
491	START	Y_J	impurities	ASH	0.0000000000000000E+00	{~~}
492	START	M	condenser	7	0.8526899202586889E-01	{~~}
493	START	H	condenser	7	-0.4624908439609421E+04	{~~}
494	START	M	condenser	8	-0.8320484335731924E-01	{~~}
495	START	P		8	0.9731000000000021E+00	{~~}
496	START	H	condenser	8	-0.4466561290262782E+04	{~~}
497	START	M	condenser	96	-0.2064148668549664E-02	{~~}
498	START	P		96	0.9731000000000021E+00	{~~}
499	START	H	condenser	96	-0.1576166949955456E+05	{~~}
500	START	M	condenser	83	0.4691527326491080E-01	{~~}
501	START	P		83	0.1013000000000002E+01	{~~}
502	START	H	condenser	83	-0.1584524528596514E+05	{~~}
503	START	M	condenser	84	-0.4691527326491080E-01	{~~}
504	START	P		84	0.1008000000000002E+01	{~~}
505	START	H	condenser	84	-0.1563608779686839E+05	{~~}
506	START	Q	condenser	308	0.0000000000000000E+00	{~~}
507	START	Y_J	dry_PG	H2	0.2614256920940560E+00	{~~}
508	START	Y_J	dry_PG	O2	0.0000000000000000E+00	{~~}
509	START	Y_J	dry_PG	N2	0.2983436780648677E+00	{~~}
510	START	Y_J	dry_PG	CO	0.1814672080223557E+00	{~~}
511	START	Y_J	dry_PG	NO	0.0000000000000000E+00	{~~}
512	START	Y_J	dry_PG	CO2	0.1178726473723852E+00	{~~}
513	START	Y_J	dry_PG	H2O-G	0.1269270417636808E+00	{~~}
514	START	Y_J	dry_PG	NH3	0.0000000000000000E+00	{~~}
515	START	Y_J	dry_PG	H2S	0.0000000000000000E+00	{~~}
516	START	Y_J	dry_PG	SO2	0.0000000000000000E+00	{~~}
517	START	Y_J	dry_PG	CH4	0.1041631550849633E-01	{~~}
518	START	Y_J	dry_PG	C2H6	0.0000000000000000E+00	{~~}
519	START	Y_J	dry_PG	C3H8	0.0000000000000000E+00	{~~}
520	START	Y_J	dry_PG	C4H10-N	0.0000000000000000E+00	{~~}
521	START	Y_J	dry_PG	C4H10-I	0.0000000000000000E+00	{~~}
522	START	Y_J	dry_PG	C5H12	0.0000000000000000E+00	{~~}
523	START	Y_J	dry_PG	C6H14	0.0000000000000000E+00	{~~}
524	START	Y_J	dry_PG	C7H16	0.0000000000000000E+00	{~~}
525	START	Y_J	dry_PG	C8H18	0.0000000000000000E+00	{~~}
526	START	Y_J	dry_PG	C2H4	0.0000000000000000E+00	{~~}
527	START	Y_J	dry_PG	C3H6	0.0000000000000000E+00	{~~}
528	START	Y_J	dry_PG	C5H10	0.0000000000000000E+00	{~~}
529	START	Y_J	dry_PG	C6H12-1	0.0000000000000000E+00	{~~}
530	START	Y_J	dry_PG	C7H14	0.0000000000000000E+00	{~~}

DNA Input for MGT scenario

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531	START Y_J	dry_PG	C2H2	0.0000000000000000E+00	{~~}
532	START Y_J	dry_PG	C6H6	0.0000000000000000E+00	{~~}
533	START Y_J	dry_PG	C6H12-C	0.0000000000000000E+00	{~~}
534	START Y_J	dry_PG	C	0.0000000000000000E+00	{~~}
535	START Y_J	dry_PG	S	0.0000000000000000E+00	{~~}
536	START Y_J	dry_PG	NO2	0.0000000000000000E+00	{~~}
537	START Y_J	dry_PG	HCN	0.0000000000000000E+00	{~~}
538	START Y_J	dry_PG	COS	0.0000000000000000E+00	{~~}
539	START Y_J	dry_PG	N2O	0.0000000000000000E+00	{~~}
540	START Y_J	dry_PG	NO3	0.0000000000000000E+00	{~~}
541	START Y_J	dry_PG	SO3	0.0000000000000000E+00	{~~}
542	START Y_J	dry_PG	AR	0.3547417174160010E-02	{~~}
543	START M	PGcompressor	8	0.8320484335731924E-01	{~~}
544	START H	PGcompressor	8	-0.4466561290262782E+04	{~~}
545	START M	PGcompressor	9	-0.8320484335731924E-01	{~~}
546	START P		9	0.3750000000000000E+01	{~~}
547	START H	PGcompressor	9	-0.4199072570137568E+04	{~~}
548	START Q	PGcompressor	309	-0.4542113685279208E+00	{~~}
549	START W	PGcompressor	117	0.2271056842639615E+02	{~~}
550	START M	aircompressor	31	0.1018083234123910E+01	{~~}
551	START P		31	0.1013000000000000E+01	{~~}
552	START H	aircompressor	31	-0.9883454496688249E+02	{~~}
553	START M	aircompressor	32	-0.1018083234123910E+01	{~~}
554	START P		32	0.3760000000000000E+01	{~~}
555	START H	aircompressor	32	0.7718226301745642E+02	{~~}
556	START Q	aircompressor	312	-0.3657137982303304E+01	{~~}
557	START W	aircompressor	117	0.1828568991151661E+03	{~~}
558	START M	burner	33	0.1018083234123910E+01	{~~}
559	START P		33	0.3750000000000000E+01	{~~}
560	START H	burner	33	0.4838361573740053E+03	{~~}
561	START M	burner	9	0.8320484335731924E-01	{~~}
562	START H	burner	9	-0.4199072570137567E+04	{~~}
563	START M	burner	41	-0.1101288077481229E+01	{~~}
564	START P		41	0.3747652500000000E+01	{~~}
565	START H	burner	41	0.1300316487295679E+03	{~~}
566	START Q	burner	316	0.0000000000000000E+00	{~~}
567	START ZA	burner	1	0.7899556968713444E+01	{~~}
568	START Y_J	FLUE_GAS	O2	0.1671258083618115E+00	{~~}
569	START Y_J	FLUE_GAS	N2	0.7425665022970938E+00	{~~}
570	START Y_J	FLUE_GAS	NO	0.0000000000000000E+00	{~~}
571	START Y_J	FLUE_GAS	CO2	0.3124559018208463E-01	{~~}
572	START Y_J	FLUE_GAS	H2O-G	0.5022354879730917E-01	{~~}
573	START Y_J	FLUE_GAS	SO2	0.0000000000000000E+00	{~~}
574	START Y_J	FLUE_GAS	NO2	0.0000000000000000E+00	{~~}
575	START Y_J	FLUE_GAS	AR	0.8838550361702892E-02	{~~}
576	START M	GT	41	0.1101288077481229E+01	{~~}
577	START H	GT	41	0.1300316487295679E+03	{~~}
578	START M	GT	42	-0.1101288077481229E+01	{~~}
579	START P		42	0.1033000000000000E+01	{~~}
580	START H	GT	42	-0.1851504231204904E+03	{~~}
581	START W	GT	117	-0.3471062579643006E+03	{~~}
582	START E	generator	217	-0.1344618509016015E+03	{~~}
583	START Q	generator	317	-0.7076939521136913E+01	{~~}
584	START W	generator	117	0.1415387904227384E+03	{~~}
585	START M	recuperator	42	0.1101288077481229E+01	{~~}
586	START H	recuperator	42	-0.1851504231204904E+03	{~~}
587	START M	recuperator	43	-0.1101288077481229E+01	{~~}
588	START P		43	0.1023000000000000E+01	{~~}
589	START H	recuperator	43	-0.5610806818793795E+03	{~~}
590	START M	recuperator	32	0.1018083234123910E+01	{~~}
591	START H	recuperator	32	0.7718226301745642E+02	{~~}
592	START M	recuperator	33	-0.1018083234123910E+01	{~~}
593	START H	recuperator	33	0.4838361573740053E+03	{~~}
594	START Q	recuperator	318	0.0000000000000000E+00	{~~}
595	START ZA	recuperator	1	0.4140075119355976E+03	{~~}
596	START M	exhaustcooler	43	0.1101288077481229E+01	{~~}
597	START H	exhaustcooler	43	-0.5610806818793795E+03	{~~}
598	START M	exhaustcooler	44	-0.1101288077481229E+01	{~~}
599	START P		44	0.1013000000000000E+01	{~~}
600	START H	exhaustcooler	44	-0.7510747147930945E+03	{~~}
601	START M	exhaustcooler	85	0.1000385710041053E+01	{~~}
602	START P		85	0.1013000000000000E+01	{~~}
603	START H	exhaustcooler	85	-0.1584524528596514E+05	{~~}
604	START M	exhaustcooler	86	-0.1000385710041053E+01	{~~}
605	START P		86	0.1008000000000000E+01	{~~}
606	START H	exhaustcooler	86	-0.1563608779686839E+05	{~~}

```
607 START Q      exhaustcooler      319  0.0000000000000000E+00  {~~}
608 START ZA     exhaustcooler      1    0.2092381632404501E+03  {~~}
609 C ~~~~~
~~~~~
610 C ~~ End of generated initial guesses.
611 C ~~~~~
~~~~~
end
```

DNA Output for MGT scenario

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1 Biomass gasification (Viking) + MGT incl. recuperation

2 RUN NUMBER 1

3

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5

6 ALGEBRAIC VARIABLES

7	NO	TO	MEDIA	M	T	P	H	ENERGY	X	S	V	U
8	DE	COMPONENT		[kg/s]	[C]	[bar]	[kJ/kg]	[kJ/s]		[kJ/kg K]	[m3/kg]	[kJ/kg]
9	-----											
10	1	Dryer	Wood	0.04	15.00	-	-8621.6	4.991E+02	-	0.4612	-	-8621.6
11	64	Dryer	STEAM-HF	0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2
12	2	Dryer	DryWood	-0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1
13	61	Dryer	STEAM-HF	-0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1
14	301	Dryer	HEAT					0.000E+00				
15	2	Gasifier	DryWood	0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1
16	26	Gasifier	STEAM-HF	0.00	150.00	1.003	-13194.5		-	11.1292	1.9309	-13388.2
17	74	Gasifier	humid_air	0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7
18	3	Gasifier	raw_PG	-0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1
19	99	Gasifier	Ash	0.00	800.00	-	-4308.0		-	0.0000	-	-4308.0
20	302	Gasifier	HEAT					0.000E+00				
21	3	airpreheat	raw_PG	0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1
22	4	airpreheat	raw_PG	-0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7
23	72	airpreheat	STANDARD_AIR	0.04	15.00	1.008	-98.8		-	6.8668	0.8237	-181.9
24	73	airpreheat	STANDARD_AIR	-0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1
25	303	airpreheat	HEAT					0.000E+00				
26	4	steamheater	raw_PG	0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7
27	5	steamheater	raw_PG	-0.09	259.48	0.988	-4375.3		-	9.7468	2.0710	-4579.9
28	63	steamheater	STEAM-HF	0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
29	64	steamheater	STEAM-HF	-0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2
30	304	steamheater	HEAT					0.000E+00				
31	61	steamblower	STEAM-HF	0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1
32	62	steamblower	STEAM-HF	-0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
33	305	steamblower	HEAT					-1.409E-02				
34	105	steamblower	MECH_POWER					7.044E-01				
35	62	split1	STEAM-HF	0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
36	63	split1	STEAM-HF	-0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
37	69	split1	STEAM-HF	-0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
38	73	mix1	STANDARD_AIR	0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1
39	69	mix1	STEAM-HF	0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
40	74	mix1	humid_air	-0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7
41	5	gascooler	raw_PG	0.09	259.48	0.988	-4375.3		-	9.7468	2.0710	-4579.9
42	6	gascooler	cold_PG	-0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1
43	98	gascooler	STEAM-HF	0.00	90.00	0.983	-15594.1		-	4.7085	0.0010	-15594.2
44	81	gascooler	STEAM-HF	0.10	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3
45	82	gascooler	STEAM-HF	-0.10	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
46	306	gascooler	HEAT					0.000E+00				
47	6	gasclean	cold_PG	0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1
48	7	gasclean	clean_PG	-0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4
49	97	gasclean	impurities	0.00	90.00	0.978	-535.6		-	6.2438	0.9059	-624.2
50	307	gasclean	HEAT					0.000E+00				
51	7	condenser	clean_PG	0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4
52	8	condenser	dry_PG	-0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1
53	96	condenser	STEAM-HF	0.00	50.01	0.973	-15761.7		-	4.2198	0.0010	-15761.7
54	83	condenser	STEAM-HF	0.05	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3

DNA Output for MGT scenario

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54	84	condenser	STEAM-HF	-0.05	80.00	1.008	-15636.1	-	4.5912	0.0010	-15636.2
56	308	condenser	HEAT				0.000E+00				
57	8	PGcompressor	dry_PG	0.08	50.00	0.973	-4466.6	-	8.9598	1.2694	-4590.1
58	9	PGcompressor	dry_PG	-0.08	234.69	3.750	-4199.1	-	9.0977	0.5176	-4393.2
59	309	PGcompressor	HEAT				-4.542E-01				
60	117	PGcompressor	MECH_POWER				2.271E+01				
61	31	aircompressor	STANDARD_AIR	1.02	15.00	1.013	-98.8	-	6.8653	0.8196	-181.9
62	32	aircompressor	STANDARD_AIR	-1.02	188.08	3.760	77.2	-	6.9655	0.3535	-55.7
63	312	aircompressor	HEAT				-3.657E+00				
64	117	aircompressor	MECH_POWER				1.829E+02				
65	42	recuperator	FLUE_GAS	1.10	635.23	1.033	-185.2	-	8.1694	2.5401	-447.5
66	43	recuperator	FLUE_GAS	-1.10	299.69	1.023	-561.1	-	7.6572	1.6175	-726.6
67	32	recuperator	STANDARD_AIR	1.02	188.08	3.760	77.2	-	6.9655	0.3535	-55.7
68	33	recuperator	STANDARD_AIR	-1.02	568.16	3.750	483.8	-	7.6068	0.6464	241.4
69	318	recuperator	HEAT				0.000E+00				
70	33	burner	STANDARD_AIR	1.02	568.16	3.750	483.8	-	7.6068	0.6464	241.4
71	9	burner	dry_PG	0.08	234.69	3.750	-4199.1	-	9.0977	0.5176	-4393.2
72	41	burner	FLUE_GAS	-1.10	900.00	3.748	130.0	-	8.1014	0.9042	-208.8
73	316	burner	HEAT				0.000E+00				
74	41	GT	FLUE_GAS	1.10	900.00	3.748	130.0	-	8.1014	0.9042	-208.8
75	42	GT	FLUE_GAS	-1.10	635.23	1.033	-185.2	-	8.1694	2.5401	-447.5
76	117	GT	MECH_POWER				-3.471E+02				
77	217	generator	ELECT_POWER				-1.345E+02				
78	317	generator	HEAT				-7.077E+00				
79	117	generator	MECH_POWER				1.415E+02				
80	43	exhaustcooler	FLUE_GAS	1.10	299.69	1.023	-561.1	-	7.6572	1.6175	-726.6
81	44	exhaustcooler	FLUE_GAS	-1.10	120.02	1.013	-751.1	-	7.2625	1.1211	-864.6
82	85	exhaustcooler	STEAM-HF	1.00	30.02	1.013	-15845.2	-	3.9530	0.0010	-15845.3
83	86	exhaustcooler	STEAM-HF	-1.00	80.00	1.008	-15636.1	-	4.5912	0.0010	-15636.2
84	319	exhaustcooler	HEAT				0.000E+00				
85	-----										
86											
87											
88	EXERGY										
89											
90	NO	TO	MEDIA	E_PH	E_CH	E	EX_PH	EX_CH	EX		
91	DE	COMPONENT		[kJ/kg]	[kJ/kg]	[kJ/kg]	[kJ/s]	[kJ/s]	[kJ/s]		
92	-----										
93	1	Dryer	Wood	0.00	13311.33	13311.33	0.00	572.39	572.39		
94	64	Dryer	STEAM-HF	660.71	-	660.71	132.17	-	132.17		
95	2	Dryer	DryWood	-54.56	18651.57	18597.01	1.67	-572.39	-570.71		
96	61	Dryer	STEAM-HF	583.11	-	583.11	-123.83	-	-123.83		
97	301	Dryer	HEAT	-	-	-	0.00	0.00	0.00		
98	2	Gasifier	DryWood	-54.56	18651.57	18597.01	-1.67	572.39	570.71		
99	26	Gasifier	STEAM-HF	584.41	-	584.41	0.00	-	0.00		
100	74	Gasifier	humid_air	310.33	66.40	376.73	17.02	3.64	20.66		
101	3	Gasifier	raw_PG	644.70	5438.32	6083.02	-54.98	-463.75	-518.73		
102	99	Gasifier	Ash	785.00	-	785.00	-0.21	-	-0.21		
103	302	Gasifier	HEAT	-	-	-	0.00	0.00	0.00		
104	3	airpreheat	raw_PG	644.70	5438.32	6083.02	54.98	463.75	518.73		
105	4	airpreheat	raw_PG	358.65	5438.32	5796.96	-30.58	-463.75	-494.34		
106	72	airpreheat	STANDARD_AIR	0.66	3.73	4.39	0.03	0.16	0.19		
107	73	airpreheat	STANDARD_AIR	427.84	3.73	431.57	-18.20	-0.16	-18.36		

DNA Output for MGT scenario

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108	303	airpreheat	HEAT		-		-		-		0.00		0.00		0.00
109	4	steamheater	raw_PG		358.65		5438.32		5796.96		30.58		463.75		494.34
110	5	steamheater	raw_PG		97.80		5438.32		5536.12		-8.34		-463.75		-472.09
111	63	steamheater	STEAM-HF		585.47		-		585.47		117.12		-		117.12
112	64	steamheater	STEAM-HF		660.71		-		660.71		-132.17		-		-132.17
113	304	steamheater	HEAT		-		-		-		0.00		0.00		0.00
114	61	steamblower	STEAM-HF		583.11		-		583.11		123.83		-		123.83
115	62	steamblower	STEAM-HF		585.47		-		585.47		-124.33		-		-124.33
116	305	steamblower	HEAT		-		-		-		0.00		0.00		0.00
117	105	steamblower	MECH_POWER		-		-		-		0.70		0.00		0.70
118	62	split1	STEAM-HF		585.47		-		585.47		124.33		-		124.33
119	63	split1	STEAM-HF		585.47		-		585.47		-117.12		-		-117.12
120	69	split1	STEAM-HF		585.47		-		585.47		-7.21		-		-7.21
121	73	mix1	STANDARD_AIR		427.84		3.73		431.57		18.20		0.16		18.36
122	69	mix1	STEAM-HF		585.47		-		585.47		7.21		-		7.21
123	74	mix1	humid_air		310.33		66.40		376.73		-17.02		-3.64		-20.66
124	5	gascooler	raw_PG		97.80		5438.32		5536.12		8.34		463.75		472.09
125	6	gascooler	cold_PG		10.04		5438.32		5448.36		-0.86		-463.75		-464.61
126	98	gascooler	STEAM-HF		34.93		-		34.93		0.00		-		0.00
127	81	gascooler	STEAM-HF		1.49		-		1.49		0.15		-		0.15
128	82	gascooler	STEAM-HF		26.73		-		26.73		-2.72		-		-2.72
129	306	gascooler	HEAT		-		-		-		0.00		0.00		0.00
130	6	gasclean	cold_PG		10.04		5438.32		5448.36		0.86		463.75		464.61
131	7	gasclean	clean_PG		9.49		5437.03		5446.52		-0.81		-463.61		-464.42
132	97	gasclean	impurities		6.93		23829.09		23836.02		0.00		-0.15		-0.15
133	307	gasclean	HEAT		-		-		-		0.00		0.00		0.00
134	7	condenser	clean_PG		9.49		5437.03		5446.52		0.81		463.61		464.42
135	8	condenser	dry_PG		-0.23		5566.16		5565.93		0.02		-463.13		-463.11
136	96	condenser	STEAM-HF		8.19		-		8.19		-0.02		-		-0.02
137	83	condenser	STEAM-HF		1.49		-		1.49		0.07		-		0.07
138	84	condenser	STEAM-HF		26.73		-		26.73		-1.25		-		-1.25
139	308	condenser	HEAT		-		-		-		0.00		0.00		0.00
140	8	PGcompressor	dry_PG		-0.23		5566.16		5565.93		-0.02		463.13		463.11
141	9	PGcompressor	dry_PG		227.52		5566.16		5793.68		-18.93		-463.13		-482.06
142	309	PGcompressor	HEAT		-		-		-		0.00		0.00		0.00
143	117	PGcompressor	MECH_POWER		-		-		-		22.71		0.00		22.71
144	31	aircompressor	STANDARD_AIR		1.07		3.73		4.81		1.09		3.80		4.89
145	32	aircompressor	STANDARD_AIR		148.24		3.73		151.97		-150.92		-3.80		-154.72
146	312	aircompressor	HEAT		-		-		-		0.00		0.00		0.00
147	117	aircompressor	MECH_POWER		-		-		-		182.86		0.00		182.86
148	42	recuperator	FLUE_GAS		321.66		15.16		336.82		354.24		16.69		370.93
149	43	recuperator	FLUE_GAS		93.34		15.16		108.49		-102.79		-16.69		-119.48
150	32	recuperator	STANDARD_AIR		148.24		3.73		151.97		150.92		3.80		154.72
151	33	recuperator	STANDARD_AIR		370.10		3.73		373.84		-376.80		-3.80		-380.60
152	318	recuperator	HEAT		-		-		-		0.00		0.00		0.00
153	33	burner	STANDARD_AIR		370.10		3.73		373.84		376.80		3.80		380.60
154	9	burner	dry_PG		227.52		5566.16		5793.68		18.93		463.13		482.06
155	41	burner	FLUE_GAS		656.45		15.16		671.61		-722.94		-16.69		-739.63
156	316	burner	HEAT		-		-		-		0.00		0.00		0.00
157	41	GT	FLUE_GAS		656.45		15.16		671.61		722.94		16.69		739.63
158	42	GT	FLUE_GAS		321.66		15.16		336.82		-354.24		-16.69		-370.93
159	117	GT	MECH_POWER		-		-		-		-347.11		0.00		-347.11
160	217	generator	ELECT_POWER		-		-		-		-134.46		0.00		-134.46
161	317	generator	HEAT		-		-		-		0.00		0.00		0.00

DNA Output for MGT scenario

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161
162 117 |generator      |MECH_POWER |      -      |      -      |      -      |    141.54 |      0.00 |    141.54|
163 43 |exhaustcooler    |FLUE_GAS  |    93.34 |    15.16 |    108.49|    102.79 |    16.69 |    119.48|
164 44 |exhaustcooler    |FLUE_GAS  |    17.07 |    15.16 |    32.23|    -18.80 |   -16.69 |   -35.49|
165 85 |exhaustcooler    |STEAM-HF  |     1.49 |      -      |     1.49|     1.50 |      -      |     1.50|
166 86 |exhaustcooler    |STEAM-HF  |    26.73 |      -      |    26.73|   -26.74 |      -      |   -26.74|
167 319 |exhaustcooler    |HEAT      |      -      |      -      |      -      |     0.00 |     0.00 |     0.00|
168 -----
169
170      ELEC. POWER PRODUCTION =      134.4619 kW
171      TOTAL POWER CONSUMPTION =         0.7044 kW
172      NET POWER PRODUCTION   =      133.7575 kW
173      FUEL CONSUMPTION (LHV) =      499.1161 kJ/s
174      FUEL CONSUMPTION (HHV) =      572.3872 kJ/s
175      THERMAL EFFICIENCY (LHV)=         0.2680
176      THERMAL EFFICIENCY (HHV)=         0.2337
177
178      MAXIMUM RELATIVE ERROR = 8.9184E-13
179      COMPUTER ACCURACY      = 1.0842E-19
180
181
182
183      IDEAL GAS COMPOSITION (MOLAR BASE):
184
185      |humid_air |raw_PG      |STANDARD_AIR|cold_PG      |clean_PG      |
186 -----
187 HYDROGEN      | 0.0000E+00 | 0.2538E+00 | 0.0000E+00 | 0.2538E+00 | 0.2538E+00 |
188 OXYGEN        | 0.1418E+00 | 0.0000E+00 | 0.2075E+00 | 0.0000E+00 | 0.0000E+00 |
189 NITROGEN      | 0.5281E+00 | 0.2897E+00 | 0.7729E+00 | 0.2897E+00 | 0.2897E+00 |
190 CARBON MONOXIDE | 0.0000E+00 | 0.1762E+00 | 0.0000E+00 | 0.1762E+00 | 0.1762E+00 |
191 CARBON DIOXIDE | 0.2050E-03 | 0.1144E+00 | 0.3000E-03 | 0.1144E+00 | 0.1144E+00 |
192 WATER (I.G.)  | 0.3236E+00 | 0.1523E+00 | 0.1010E-01 | 0.1523E+00 | 0.1523E+00 |
193 HYDROGEN SULFIDE| 0.0000E+00 | 0.4616E-04 | 0.0000E+00 | 0.4616E-04 | 0.0000E+00 |
194 METHANE        | 0.0000E+00 | 0.1011E-01 | 0.0000E+00 | 0.1011E-01 | 0.1011E-01 |
195 ARGON          | 0.6286E-02 | 0.3444E-02 | 0.9200E-02 | 0.3444E-02 | 0.3444E-02 |
196 -----
197 MEAN MOLE MASS| 0.2542E+02 | 0.2164E+02 | 0.2885E+02 | 0.2164E+02 | 0.2164E+02 |
198 NET CALORI VALUE| 0.0000E+00 | 0.5516E+04 | 0.0000E+00 | 0.5516E+04 | 0.5515E+04 |
199 GRS CALORI VALUE| 0.0000E+00 | 0.1148E+05 | 0.0000E+00 | 0.1148E+05 | 0.1148E+05 |
200 -----
201
202      IDEAL GAS COMPOSITION (MOLAR BASE):
203
204      |impurities |dry_PG      |FLUE_GAS      |
205 -----
206 HYDROGEN      | 0.0000E+00 | 0.2614E+00 | 0.0000E+00 |
207 OXYGEN        | 0.0000E+00 | 0.0000E+00 | 0.1671E+00 |
208 NITROGEN      | 0.0000E+00 | 0.2983E+00 | 0.7426E+00 |
209 CARBON MONOXIDE | 0.0000E+00 | 0.1815E+00 | 0.0000E+00 |
210 CARBON DIOXIDE | 0.0000E+00 | 0.1179E+00 | 0.3125E-01 |
211 WATER (I.G.)  | 0.0000E+00 | 0.1269E+00 | 0.5022E-01 |
212 HYDROGEN SULFIDE| 0.1000E+01 | 0.0000E+00 | 0.0000E+00 |
213 METHANE        | 0.0000E+00 | 0.1042E-01 | 0.0000E+00 |
214 ARGON          | 0.0000E+00 | 0.3547E-02 | 0.8839E-02 |
```


DNA Output for MGT scenario

5/6

```
215 -----
216 MEAN MOLE MASS| 0.3408E+02 | 0.2175E+02 | 0.2878E+02 |
217 NET CALORI VALUE| 0.1521E+05 | 0.5652E+04 | 0.0000E+00 |
218 GRS CALORI VALUE| 0.1650E+05 | 0.1172E+05 | 0.0000E+00 |
219 -----
220
221 NON-IDEAL FLUID AND SOLID COMPOSITION (MASS BASE):
222
223 |Wood      |DryWood    |Ash        |
224 -----
225 HYDROGEN      | 0.4204E-01 | 0.5890E-01 | 0.0000E+00 |
226 OXYGEN        | 0.2976E+00 | 0.4171E+00 | 0.0000E+00 |
227 NITROGEN      | 0.1153E-02 | 0.1615E-02 | 0.0000E+00 |
228 CARBON (SOLID) | 0.3309E+00 | 0.4636E+00 | 0.0000E+00 |
229 SULFUR (SOLID) | 0.1356E-03 | 0.1900E-03 | 0.0000E+00 |
230 WATER (LIQUID) | 0.3220E+00 | 0.5000E-01 | 0.0000E+00 |
231 ASHES         | 0.6170E-02 | 0.8645E-02 | 0.1000E+01 |
232 -----
233 MEAN MOLE MASS| 0.1321E+02 | 0.1193E+02 | 0.7600E+02 |
234 NET CALORI VALUE| 0.1161E+05 | 0.1724E+05 | 0.0000E+00 |
235 GRS CALORI VALUE| 0.1331E+05 | 0.1865E+05 | 0.0000E+00 |
236 -----
237
238 MEDIUM 97 : WATER FOR GAS APP
239 MEDIUM 300 : HEAT
240 MEDIUM 301 : PRODUCT HEAT
241
242
243 NUMBER OF CLOSED INTERNAL LOOPS IN THE SYSTEM: 0
244
245
246
247
248
249 SOLUTION FOR THE INDEPENDENT ALGEBRAIC VARIABLES :
250
251
252 VARIABLE NO | COMPONENT | NAME | VALUE |
253 -----
254 1 |Gasifier |MULTIPLIER H| 0.8501E+05 |
255 2 |Gasifier |MULTIPLIER C| 0.4364E+05 |
256 3 |Gasifier |MULTIPLIER N| 0.1173E+06 |
257 4 |Gasifier |MULTIPLIER O| 0.3125E+06 |
258 5 |Gasifier |MULTIPLIER S| 0.1828E+06 |
259 6 |Gasifier |MULTIPL Ar | 0.2292E+06 |
260 7 |Gasifier |GIBBS ENERGY| -.3280E+06 |
261 1 |airpreheat |Transferred | 0.3503E+02 |
262 1 |steamheater |Transferred | 0.3894E+02 |
263 1 |recuperator |Transferred | 0.4140E+03 |
264 1 |burner |Lambda | 0.7900E+01 |
265 1 |exhaustcooler |Transferred | 0.2092E+03 |
266 -----
267
268 =====
```

DNA Output for MGT scenario

6/6

```
269 #####  
end
```

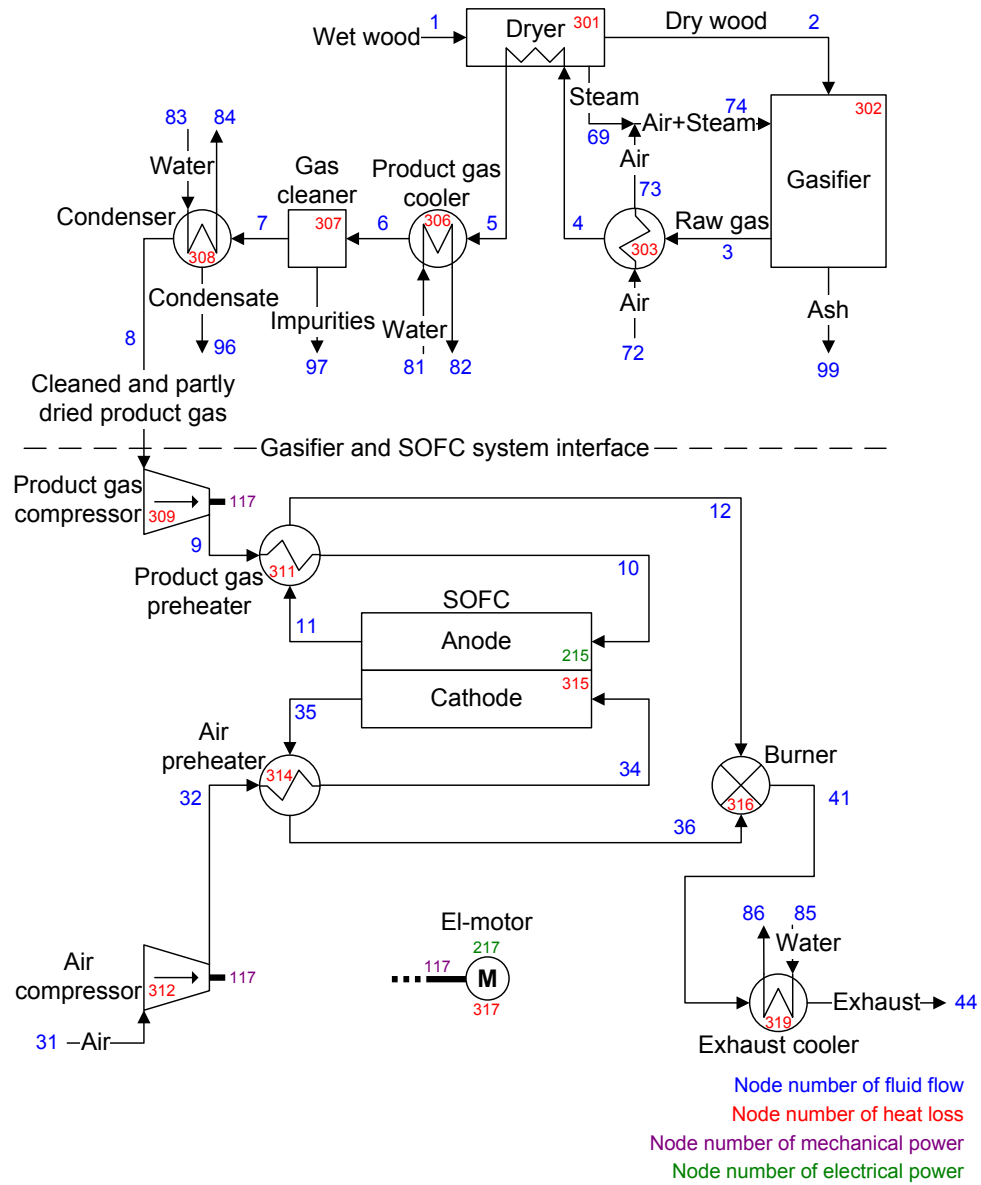
Appendix D SOFC PLANT MODEL LISTING

Included in this Appendix are:

- Flow sheet of SOFC scenario with node numbers (1 page)
- DNA Input for SOFC scenario (9 pages)
- DNA Output for SOFC scenario (6 pages)

The input and output data only represent one simulation using the reference conditions.

Flow sheet of SOFC scenario with node numbers



DNA Input for SOFC scenario

1/9

```
1 title Biomass gasification (Viking) + SOFC
2 C Wood is dried and gasified. The gasification is atmospheric,
3 C based on air, and almost reaches equilibrium. The produced
4 C product gas (PG) composition and the cold gas efficiency is
5 C similar to that from the Viking gasifier.
6 C Power and heat production by an SOFC system.
7
8
9 C #####
10 C #####
11 C #####
12 C -----GASIFIER PART-----
13 C #####
14 C #####
15 C #####
16
17 C ##Media##
18 media 1 Wood 2 DryWood
19 media 73 STANDARD_AIR 3 raw_PG 99 Ash
20
21 C ##Fuel composition##
22 solid Wood C 0.488 H .062 O .439 S .0002 N 0.0017 ASH .0091
23 + LHV 18280 CP 1.35 MOI .322
24 C [Ahrenfeldt, J. et al., Energy & Fuels 2006, 20, 2672-2680] without Cl.
25
26
27
28 C #####
29 C -----DRYER-----
30 C #####
31 struc Dryer DRYER_03 1 64 2 61 301 0.05 0.005
32
33 C Fuel input (plant size):
34 addco m Dryer 1 0.043
35
36 addco t Dryer 1 15 p 1 1.013
37 addco p 2 1.008 t Dryer 2 150
38 addco q Dryer 301 0
39
40
41
42 C #####
43 C -----GASIFIER-----
44 C #####
45 struc Gasifier GASIFI_3 8 2 26 74 3 99 302 1 3 4 6 7 9 11 36 /
46 0.998 800 0.005 0 1.0 0.01
47 C Variable constitution parameter: Number of calculated gas components 8
48 C Nodes: Inlet fuel 2; inlet water 26; inlet air 74; outlet PG 3,
49 C outlet ash 99, heat loss 302
50 C Integer Parameters: Calculated gas compounds H2 (1), N2 (3), CO (4),
51 C CO2 (6), H2O (7), H2S (9), CH4 (11), Ar (36)
52 C Real parameter: Pressure 1 bar, Eq. temperature 800 degC, Pressure loss 0,
53 C Water-to-fuel ratio 0, carbon conversion factor 1,
54 C non-equilibrium methane 0.01.
55
56 addco t Gasifier 3 800
57 addco t Gasifier 26 150
58 addco p 99 1.013
59 addco q Gasifier 302 0
60
61
62
63 C #####
64 C -----GASIFIER AIR PREHEATER-----
65 C #####
66 struc airpreheat heatex_2 3 4 72 73 303 20 0.005 0.005
67 addco t airpreheat 72 15
68 addco q airpreheat 303 0
69
70
71
72 C #####
73 C -----STEAM HEATER-----
74 C #####
75 struc steamheater heatex_1 4 5 63 64 304 0.005 0.005
76
```

DNA Input for SOFC scenario

2/9

```
77 media 63 STEAM-HF
78
79 addco t steamheater 64 250
80 addco q steamheater 304 0
81
82
83
84 C #####
85 C -----STEAM BLOWER-----
86 C #####
87 struc steamblower COMPRE_1 61 62 305 105 0.6 0.98
88
89
90
91 C #####
92 C -----SPLITTER-----
93 C #####
94 struc split1 SPLITTER 62 63 69
95
96
97
98 C #####
99 C -----MIXER-----
100 C #####
101 struc mix1 MIXER_02 73 69 74
102
103 media 74 humid_air
104
105
106
107 C #####
108 C -----GAS COOLER-----
109 C #####
110 struc gascooler GASCOOL1 5 6 98 81 82 306 0.005 0.005
111
112 media 81 STEAM-HF 6 cold_PG
113
114 addco t gascooler 6 90
115 addco t gascooler 81 30 p 81 1.013
116 addco t gascooler 82 80
117 addco q gascooler 306 0
118
119
120
121 C #####
122 C -----GAS CLEANING-----
123 C #####
124 struc gasclean GASCLE_1 6 7 97 307 0.0049
125 C Pressure loss is taken from paper about Viking
126
127 media 7 clean_PG 97 impurities
128
129 addco q gasclean 307 0
130
131
132
133 C #####
134 C -----CONDENSER-----
135 C #####
136 struc condenser GASCOOL1 7 8 96 83 84 308 0.005 0.005
137
138 media 83 STEAM-HF 8 dry_PG
139
140 addco t condenser 8 50
141 addco t condenser 83 30 p 83 1.013
142 addco t condenser 84 80
143 addco q condenser 308 0
144
145
146
147 C #####
148 C #####
149 C #####
150 C -----SOFC PART-----
151 C #####
152 C #####
```

DNA Input for SOFC scenario

3/9

```
153 C #####
154
155 media 11 USED_FUEL 35 USED_AIR
156
157
158
159 C #####
160 C -----PRODUCT GAS COMPRESSOR-----
161 C #####
162 struc PGcompressor compre_1 8 9 309 117 0.6 0.98
163 C Isentropic efficiency from L. Fryda et al. (2008)
164
165
166
167 C #####
168 C -----PRODUCT GAS PREHEATING-----
169 C #####
170 struc PGpreheat heatex_2 11 12 9 10 311 150 0.005 0.005
171 addco q PGpreheat 311 0
172
173
174
175 C #####
176 C -----AIR COMPRESSOR-----
177 C #####
178 struc aircompressor compre_1 31 32 312 117 0.6 0.98
179
180 media 31 STANDARD_AIR
181 addco p 31 1.013 t aircompressor 31 15
182
183
184
185 C #####
186 C -----AIR PREHEATING-----
187 C #####
188 struc airpreheat2 heatex_2 35 36 32 34 314 200 0.01 0.01
189 addco q airpreheat2 314 0
190
191
192
193 C #####
194 C -----SOFC-----
195 C #####
196 struc sofc sofcEq0d_CBM /
197 {fuel and air inlets} 10 34 /
198 {fuel and air outlets} 11 35 /
199 {nodes for power and heat loss} 215 315 /
200 {parameters: utilization, temperature} 0.85 800 /
201 {pressure loss} 0.005 0.010 /
202 {temperature difference between anode and cathode outlet} 0 /
203 {current density [mA/cm^2]} 300 /
204 {DC to AC conversion efficiency [-]} 0.95
205
206 addco q sofc 315 0
207
208 C SOFC OPERATING PRESSURE:
209 C addco p 10 2.5
210
211
212
213 C #####
214 C -----EL-MOTOR-----
215 C #####
216 struc el-motor el-motor 217 317 117 0.95
217
218
219
220 C #####
221 C -----BURNER-----
222 C #####
223 struc burner GASBUR_3 36 12 41 316 0.999374
224
225 media 41 FLUE_GAS
226
227 addco q burner 316 0
228
```



```

229
230
231 C #####
232 C -----EXHAUST COOLING-----
233 C #####
234 struc exhaustcooler heatex_2 41 44 85 86 319 90 0.010 0.005
235
236 media 85 STEAM-HF
237
238 addco p 44 1.013
239 addco p 85 1.013 t exhaustcooler 85 30
240 addco t exhaustcooler 86 80
241 addco q exhaustcooler 319 0
242
243
244
245 C Reference conditions for exergy
246 xergy p 1 t 15
247
248
249
250
251 C ~~~~~
~~~~~
252 C ~ Start of list of generated initial guesses.
253 C ~ The values are the results of the latest simulation.
254 C ~~~~~
~~~~~
255 START M Dryer 1 0.4300000000000009E-01 {~~}
256 START P 1 0.1013000000000002E+01 {~~}
257 START H Dryer 1 -0.8621618755529553E+04 {~~}
258 START M Dryer 64 0.2000459030657089E+00 {~~}
259 START P 64 0.9980000000000021E+00 {~~}
260 START H Dryer 64 -0.1299653551379775E+05 {~~}
261 START M Dryer 2 -0.3068842105263164E-01 {~~}
262 START P 2 0.1008000000000002E+01 {~~}
263 START H Dryer 2 -0.5497059220211011E+04 {~~}
264 START M Dryer 61 -0.2123574820130773E+00 {~~}
265 START P 61 0.9930000000000021E+00 {~~}
266 START H Dryer 61 -0.1319443607829822E+05 {~~}
267 START Q Dryer 301 0.000000000000000E+00 {~~}
268 START X_J DryWood H2 0.5890000000000011E-01 {~~}
269 START X_J DryWood O2 0.4170500000000009E+00 {~~}
270 START X_J DryWood N2 0.1615000000000003E-02 {~~}
271 START X_J DryWood CO 0.000000000000000E+00 {~~}
272 START X_J DryWood NO 0.000000000000000E+00 {~~}
273 START X_J DryWood CO2 0.000000000000000E+00 {~~}
274 START X_J DryWood H2O-L 0.5000000000000009E-01 {~~}
275 START X_J DryWood NH3 0.000000000000000E+00 {~~}
276 START X_J DryWood H2S 0.000000000000000E+00 {~~}
277 START X_J DryWood SO2 0.000000000000000E+00 {~~}
278 START X_J DryWood CH4 0.000000000000000E+00 {~~}
279 START X_J DryWood C2H6 0.000000000000000E+00 {~~}
280 START X_J DryWood C3H8 0.000000000000000E+00 {~~}
281 START X_J DryWood C4H10-N 0.000000000000000E+00 {~~}
282 START X_J DryWood C4H10-I 0.000000000000000E+00 {~~}
283 START X_J DryWood C5H12 0.000000000000000E+00 {~~}
284 START X_J DryWood C6H14 0.000000000000000E+00 {~~}
285 START X_J DryWood C7H16 0.000000000000000E+00 {~~}
286 START X_J DryWood C8H18 0.000000000000000E+00 {~~}
287 START X_J DryWood C2H4 0.000000000000000E+00 {~~}
288 START X_J DryWood C3H6 0.000000000000000E+00 {~~}
289 START X_J DryWood C5H10 0.000000000000000E+00 {~~}
290 START X_J DryWood C6H12-1 0.000000000000000E+00 {~~}
291 START X_J DryWood C7H14 0.000000000000000E+00 {~~}
292 START X_J DryWood C2H2 0.000000000000000E+00 {~~}
293 START X_J DryWood C6H6 0.000000000000000E+00 {~~}
294 START X_J DryWood C6H12-C 0.000000000000000E+00 {~~}
295 START X_J DryWood C 0.4636000000000009E+00 {~~}
296 START X_J DryWood S 0.1900000000000004E-03 {~~}
297 START X_J DryWood NO2 0.000000000000000E+00 {~~}
298 START X_J DryWood HCN 0.000000000000000E+00 {~~}
299 START X_J DryWood COS 0.000000000000000E+00 {~~}
300 START X_J DryWood N2O 0.000000000000000E+00 {~~}
301 START X_J DryWood NO3 0.000000000000000E+00 {~~}
302 START X_J DryWood SO3 0.000000000000000E+00 {~~}

```

```

303 START X_J DryWood AR 0.0000000000000000E+00 {~~}
304 START X_J DryWood ASH 0.8645000000000019E-02 {~~}
305 START X_J DryWood TAR 0.0000000000000000E+00 {~~}
306 START M Gasifier 2 0.3068842105263164E-01 {~~}
307 START H Gasifier 2 -0.5497059220211011E+04 {~~}
308 START M Gasifier 26 0.0000000000000000E+00 {~~}
309 START P 26 0.10030000000000002E+01 {~~}
310 START H Gasifier 26 -0.1319450918722708E+05 {~~}
311 START M Gasifier 74 0.5485206982616303E-01 {~~}
312 START P 74 0.10030000000000002E+01 {~~}
313 START H Gasifier 74 -0.2398848478333937E+04 {~~}
314 START M Gasifier 3 -0.8527518947879467E-01 {~~}
315 START P 3 0.99800000000000021E+00 {~~}
316 START H Gasifier 3 -0.3507877913073770E+04 {~~}
317 START M Gasifier 99 -0.26530140000000006E-03 {~~}
318 START P 99 0.10130000000000002E+01 {~~}
319 START H Gasifier 99 -0.43080000000000007E+04 {~~}
320 START Q Gasifier 302 0.0000000000000000E+00 {~~}
321 START ZA Gasifier 1 0.8500945239865259E+05 {~~}
322 START ZA Gasifier 2 0.4363965291425181E+05 {~~}
323 START ZA Gasifier 3 0.1172765217993688E+06 {~~}
324 START ZA Gasifier 4 0.3124902840469579E+06 {~~}
325 START ZA Gasifier 5 0.1827651987487792E+06 {~~}
326 START ZA Gasifier 6 0.2292482774424776E+06 {~~}
327 START ZA Gasifier 7 -0.3279719879436739E+06 {~~}
328 START Y_J raw_PG H2 0.2538114658675977E+00 {~~}
329 START Y_J raw_PG O2 0.0000000000000000E+00 {~~}
330 START Y_J raw_PG N2 0.2896541868376543E+00 {~~}
331 START Y_J raw_PG CO 0.1761818347160904E+00 {~~}
332 START Y_J raw_PG NO 0.0000000000000000E+00 {~~}
333 START Y_J raw_PG CO2 0.1144395150133743E+00 {~~}
334 START Y_J raw_PG H2O-G 0.1523098114753791E+00 {~~}
335 START Y_J raw_PG NH3 0.0000000000000000E+00 {~~}
336 START Y_J raw_PG H2S 0.4615796164902312E-04 {~~}
337 START Y_J raw_PG SO2 0.0000000000000000E+00 {~~}
338 START Y_J raw_PG CH4 0.1011293223314740E-01 {~~}
339 START Y_J raw_PG NO2 0.0000000000000000E+00 {~~}
340 START Y_J raw_PG HCN 0.0000000000000000E+00 {~~}
341 START Y_J raw_PG COS 0.0000000000000000E+00 {~~}
342 START Y_J raw_PG AR 0.3444095895109989E-02 {~~}
343 START X_J Ash C 0.0000000000000000E+00 {~~}
344 START X_J Ash ASH 0.10000000000000002E+01 {~~}
345 START M airpreheat 3 0.8527518947879467E-01 {~~}
346 START H airpreheat 3 -0.3507877913073770E+04 {~~}
347 START M airpreheat 4 -0.8527518947879467E-01 {~~}
348 START P 4 0.99300000000000021E+00 {~~}
349 START H airpreheat 4 -0.3918630307677503E+04 {~~}
350 START M airpreheat 72 0.4254049087879458E-01 {~~}
351 START P 72 0.10080000000000002E+01 {~~}
352 START H airpreheat 72 -0.9883454496688249E+02 {~~}
353 START M airpreheat 73 -0.4254049087879458E-01 {~~}
354 START P 73 0.10030000000000002E+01 {~~}
355 START H airpreheat 73 0.7245454291500147E+03 {~~}
356 START Q airpreheat 303 0.0000000000000000E+00 {~~}
357 START ZA airpreheat 1 0.3502698827870192E+02 {~~}
358 START M steamheater 4 0.8527518947879467E-01 {~~}
359 START H steamheater 4 -0.3918630307677503E+04 {~~}
360 START M steamheater 5 -0.8527518947879467E-01 {~~}
361 START P 5 0.98800000000000021E+00 {~~}
362 START H steamheater 5 -0.4375257198957320E+04 {~~}
363 START M steamheater 63 0.2000459030657089E+00 {~~}
364 START P 63 0.10030000000000002E+01 {~~}
365 START H steamheater 63 -0.1319118556200298E+05 {~~}
366 START M steamheater 64 -0.2000459030657089E+00 {~~}
367 START H steamheater 64 -0.1299653551379775E+05 {~~}
368 START Q steamheater 304 0.0000000000000000E+00 {~~}
369 START ZA steamheater 1 0.3893894467499928E+02 {~~}
370 START M steamblower 61 0.2123574820130773E+00 {~~}
371 START H steamblower 61 -0.1319443607829822E+05 {~~}
372 START M steamblower 62 -0.2123574820130773E+00 {~~}
373 START P 62 0.10030000000000002E+01 {~~}
374 START H steamblower 62 -0.1319118556200298E+05 {~~}
375 START Q steamblower 305 -0.1408717256529172E-01 {~~}
376 START W steamblower 105 0.7043586282645917E+00 {~~}
377 START M split1 62 0.2123574820130773E+00 {~~}
378 START H split1 62 -0.1319118556200298E+05 {~~}

```

```

379 START M split1 63 -0.2000459030657089E+00 {~~}
380 START H split1 63 -0.1319118556200298E+05 {~~}
381 START M split1 69 -0.1231157894736844E-01 {~~}
382 START P 69 0.10030000000000002E+01 {~~}
383 START H split1 69 -0.1319118556200298E+05 {~~}
384 START M mix1 73 0.4254049087879458E-01 {~~}
385 START H mix1 73 0.7245454291500147E+03 {~~}
386 START M mix1 69 0.1231157894736844E-01 {~~}
387 START H mix1 69 -0.1319118556200299E+05 {~~}
388 START M mix1 74 -0.5485206982616303E-01 {~~}
389 START H mix1 74 -0.2398848478333937E+04 {~~}
390 START Y_J humid_air H2 0.0000000000000000E+00 {~~}
391 START Y_J humid_air O2 0.1417803964772677E+00 {~~}
392 START Y_J humid_air N2 0.5281063539146036E+00 {~~}
393 START Y_J humid_air CO 0.0000000000000000E+00 {~~}
394 START Y_J humid_air NO 0.0000000000000000E+00 {~~}
395 START Y_J humid_air CO2 0.2049837057502667E-03 {~~}
396 START Y_J humid_air H2O-G 0.3236220989260387E+00 {~~}
397 START Y_J humid_air NH3 0.0000000000000000E+00 {~~}
398 START Y_J humid_air H2S 0.0000000000000000E+00 {~~}
399 START Y_J humid_air SO2 0.0000000000000000E+00 {~~}
400 START Y_J humid_air CH4 0.0000000000000000E+00 {~~}
401 START Y_J humid_air C2H6 0.0000000000000000E+00 {~~}
402 START Y_J humid_air C3H8 0.0000000000000000E+00 {~~}
403 START Y_J humid_air C4H10-N 0.0000000000000000E+00 {~~}
404 START Y_J humid_air C4H10-I 0.0000000000000000E+00 {~~}
405 START Y_J humid_air C5H12 0.0000000000000000E+00 {~~}
406 START Y_J humid_air C6H14 0.0000000000000000E+00 {~~}
407 START Y_J humid_air C7H16 0.0000000000000000E+00 {~~}
408 START Y_J humid_air C8H18 0.0000000000000000E+00 {~~}
409 START Y_J humid_air C2H4 0.0000000000000000E+00 {~~}
410 START Y_J humid_air C3H6 0.0000000000000000E+00 {~~}
411 START Y_J humid_air C5H10 0.0000000000000000E+00 {~~}
412 START Y_J humid_air C6H12-1 0.0000000000000000E+00 {~~}
413 START Y_J humid_air C7H14 0.0000000000000000E+00 {~~}
414 START Y_J humid_air C2H2 0.0000000000000000E+00 {~~}
415 START Y_J humid_air C6H6 0.0000000000000000E+00 {~~}
416 START Y_J humid_air C6H12-C 0.0000000000000000E+00 {~~}
417 START Y_J humid_air C 0.0000000000000000E+00 {~~}
418 START Y_J humid_air S 0.0000000000000000E+00 {~~}
419 START Y_J humid_air NO2 0.0000000000000000E+00 {~~}
420 START Y_J humid_air HCN 0.0000000000000000E+00 {~~}
421 START Y_J humid_air COS 0.0000000000000000E+00 {~~}
422 START Y_J humid_air N2O 0.0000000000000000E+00 {~~}
423 START Y_J humid_air NO3 0.0000000000000000E+00 {~~}
424 START Y_J humid_air SO3 0.0000000000000000E+00 {~~}
425 START Y_J humid_air AR 0.6286166976341510E-02 {~~}
426 START Y_J humid_air ASH 0.0000000000000000E+00 {~~}
427 START Y_J humid_air TAR 0.0000000000000000E+00 {~~}
428 START Y_J humid_air CH3OH 0.0000000000000000E+00 {~~}
429 START M gascooler 5 0.8527518947879467E-01 {~~}
430 START H gascooler 5 -0.4375257198957320E+04 {~~}
431 START M gascooler 6 -0.8527518947879467E-01 {~~}
432 START P 6 0.983000000000000021E+00 {~~}
433 START H gascooler 6 -0.4624611248324039E+04 {~~}
434 START M gascooler 98 0.0000000000000000E+00 {~~}
435 START P 98 0.983000000000000021E+00 {~~}
436 START H gascooler 98 -0.1559408877861427E+05 {~~}
437 START M gascooler 81 0.1016636501943104E+00 {~~}
438 START P 81 0.101300000000000002E+01 {~~}
439 START H gascooler 81 -0.1584524528596514E+05 {~~}
440 START M gascooler 82 -0.1016636501943104E+00 {~~}
441 START P 82 0.100800000000000002E+01 {~~}
442 START H gascooler 82 -0.1563608779686839E+05 {~~}
443 START Q gascooler 306 0.0000000000000000E+00 {~~}
444 START Y_J cold_PG H2 0.2538114658675973E+00 {~~}
445 START Y_J cold_PG O2 0.0000000000000000E+00 {~~}
446 START Y_J cold_PG N2 0.2896541868376540E+00 {~~}
447 START Y_J cold_PG CO 0.1761818347160902E+00 {~~}
448 START Y_J cold_PG NO 0.0000000000000000E+00 {~~}
449 START Y_J cold_PG CO2 0.1144395150133742E+00 {~~}
450 START Y_J cold_PG H2O-G 0.1523098114753791E+00 {~~}
451 START Y_J cold_PG NH3 0.0000000000000000E+00 {~~}
452 START Y_J cold_PG H2S 0.4615796164902307E-04 {~~}
453 START Y_J cold_PG SO2 0.0000000000000000E+00 {~~}
454 START Y_J cold_PG CH4 0.1011293223314739E-01 {~~}

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455	START	Y_J	cold_PG	C2H6	0.0000000000000000E+00	{~~}
456	START	Y_J	cold_PG	C3H8	0.0000000000000000E+00	{~~}
457	START	Y_J	cold_PG	C4H10-N	0.0000000000000000E+00	{~~}
458	START	Y_J	cold_PG	C4H10-I	0.0000000000000000E+00	{~~}
459	START	Y_J	cold_PG	C5H12	0.0000000000000000E+00	{~~}
460	START	Y_J	cold_PG	C6H14	0.0000000000000000E+00	{~~}
461	START	Y_J	cold_PG	C7H16	0.0000000000000000E+00	{~~}
462	START	Y_J	cold_PG	C8H18	0.0000000000000000E+00	{~~}
463	START	Y_J	cold_PG	C2H4	0.0000000000000000E+00	{~~}
464	START	Y_J	cold_PG	C3H6	0.0000000000000000E+00	{~~}
465	START	Y_J	cold_PG	C5H10	0.0000000000000000E+00	{~~}
466	START	Y_J	cold_PG	C6H12-1	0.0000000000000000E+00	{~~}
467	START	Y_J	cold_PG	C7H14	0.0000000000000000E+00	{~~}
468	START	Y_J	cold_PG	C2H2	0.0000000000000000E+00	{~~}
469	START	Y_J	cold_PG	C6H6	0.0000000000000000E+00	{~~}
470	START	Y_J	cold_PG	C6H12-C	0.0000000000000000E+00	{~~}
471	START	Y_J	cold_PG	C	0.0000000000000000E+00	{~~}
472	START	Y_J	cold_PG	S	0.0000000000000000E+00	{~~}
473	START	Y_J	cold_PG	NO2	0.0000000000000000E+00	{~~}
474	START	Y_J	cold_PG	HCN	0.0000000000000000E+00	{~~}
475	START	Y_J	cold_PG	COS	0.0000000000000000E+00	{~~}
476	START	Y_J	cold_PG	N2O	0.0000000000000000E+00	{~~}
477	START	Y_J	cold_PG	NO3	0.0000000000000000E+00	{~~}
478	START	Y_J	cold_PG	SO3	0.0000000000000000E+00	{~~}
479	START	Y_J	cold_PG	AR	0.3444095895109983E-02	{~~}
480	START	M	gasclean	6	0.8527518947879467E-01	{~~}
481	START	H	gasclean	6	-0.4624611248324039E+04	{~~}
482	START	M	gasclean	7	-0.8526899202586889E-01	{~~}
483	START	P		7	0.9781000000000021E+00	{~~}
484	START	H	gasclean	7	-0.4624908439609422E+04	{~~}
485	START	M	gasclean	97	-0.6197452925764206E-05	{~~}
486	START	P		97	0.9781000000000021E+00	{~~}
487	START	H	gasclean	97	-0.5356408846834938E+03	{~~}
488	START	Q	gasclean	307	0.0000000000000000E+00	{~~}
489	START	Y_J	clean_PG	H2	0.2538231818282900E+00	{~~}
490	START	Y_J	clean_PG	O2	0.0000000000000000E+00	{~~}
491	START	Y_J	clean_PG	N2	0.2896675573016551E+00	{~~}
492	START	Y_J	clean_PG	CO	0.1761899672858432E+00	{~~}
493	START	Y_J	clean_PG	NO	0.0000000000000000E+00	{~~}
494	START	Y_J	clean_PG	CO2	0.1144447975519506E+00	{~~}
495	START	Y_J	clean_PG	H2O-G	0.1523168421103358E+00	{~~}
496	START	Y_J	clean_PG	CH4	0.1011339904703275E-01	{~~}
497	START	Y_J	clean_PG	NO2	0.0000000000000000E+00	{~~}
498	START	Y_J	clean_PG	AR	0.3444254874894413E-02	{~~}
499	START	Y_J	impurities	H2O-G	0.0000000000000000E+00	{~~}
500	START	Y_J	impurities	NH3	0.0000000000000000E+00	{~~}
501	START	Y_J	impurities	H2S	0.1000000000000002E+01	{~~}
502	START	Y_J	impurities	SO2	0.0000000000000000E+00	{~~}
503	START	Y_J	impurities	HCN	0.0000000000000000E+00	{~~}
504	START	Y_J	impurities	COS	0.0000000000000000E+00	{~~}
505	START	Y_J	impurities	AR	0.0000000000000000E+00	{~~}
506	START	Y_J	impurities	ASH	0.0000000000000000E+00	{~~}
507	START	M	condenser	7	0.8526899202586889E-01	{~~}
508	START	H	condenser	7	-0.4624908439609422E+04	{~~}
509	START	M	condenser	8	-0.8320484335731876E-01	{~~}
510	START	P		8	0.9731000000000021E+00	{~~}
511	START	H	condenser	8	-0.4466561290262733E+04	{~~}
512	START	M	condenser	96	-0.2064148668550151E-02	{~~}
513	START	P		96	0.9731000000000021E+00	{~~}
514	START	H	condenser	96	-0.1576166949955456E+05	{~~}
515	START	M	condenser	83	0.4691527326491761E-01	{~~}
516	START	P		83	0.1013000000000002E+01	{~~}
517	START	H	condenser	83	-0.1584524528596514E+05	{~~}
518	START	M	condenser	84	-0.4691527326491761E-01	{~~}
519	START	P		84	0.1008000000000002E+01	{~~}
520	START	H	condenser	84	-0.1563608779686839E+05	{~~}
521	START	Q	condenser	308	0.0000000000000000E+00	{~~}
522	START	Y_J	dry_PG	H2	0.2614256920940575E+00	{~~}
523	START	Y_J	dry_PG	O2	0.0000000000000000E+00	{~~}
524	START	Y_J	dry_PG	N2	0.2983436780648697E+00	{~~}
525	START	Y_J	dry_PG	CO	0.1814672080223573E+00	{~~}
526	START	Y_J	dry_PG	NO	0.0000000000000000E+00	{~~}
527	START	Y_J	dry_PG	CO2	0.1178726473723858E+00	{~~}
528	START	Y_J	dry_PG	H2O-G	0.1269270417636751E+00	{~~}
529	START	Y_J	dry_PG	NH3	0.0000000000000000E+00	{~~}
530	START	Y_J	dry_PG	H2S	0.0000000000000000E+00	{~~}

531	START Y J	dry_PG	SO2	0.0000000000000000E+00	{~~}
532	START Y J	dry_PG	CH4	0.1041631550849640E-01	{~~}
533	START Y J	dry_PG	C2H6	0.0000000000000000E+00	{~~}
534	START Y J	dry_PG	C3H8	0.0000000000000000E+00	{~~}
535	START Y J	dry_PG	C4H10-N	0.0000000000000000E+00	{~~}
536	START Y J	dry_PG	C4H10-I	0.0000000000000000E+00	{~~}
537	START Y J	dry_PG	C5H12	0.0000000000000000E+00	{~~}
538	START Y J	dry_PG	C6H14	0.0000000000000000E+00	{~~}
539	START Y J	dry_PG	C7H16	0.0000000000000000E+00	{~~}
540	START Y J	dry_PG	C8H18	0.0000000000000000E+00	{~~}
541	START Y J	dry_PG	C2H4	0.0000000000000000E+00	{~~}
542	START Y J	dry_PG	C3H6	0.0000000000000000E+00	{~~}
543	START Y J	dry_PG	C5H10	0.0000000000000000E+00	{~~}
544	START Y J	dry_PG	C6H12-1	0.0000000000000000E+00	{~~}
545	START Y J	dry_PG	C7H14	0.0000000000000000E+00	{~~}
546	START Y J	dry_PG	C2H2	0.0000000000000000E+00	{~~}
547	START Y J	dry_PG	C6H6	0.0000000000000000E+00	{~~}
548	START Y J	dry_PG	C6H12-C	0.0000000000000000E+00	{~~}
549	START Y J	dry_PG	C	0.0000000000000000E+00	{~~}
550	START Y J	dry_PG	S	0.0000000000000000E+00	{~~}
551	START Y J	dry_PG	NO2	0.0000000000000000E+00	{~~}
552	START Y J	dry_PG	HCN	0.0000000000000000E+00	{~~}
553	START Y J	dry_PG	COS	0.0000000000000000E+00	{~~}
554	START Y J	dry_PG	N2O	0.0000000000000000E+00	{~~}
555	START Y J	dry_PG	NO3	0.0000000000000000E+00	{~~}
556	START Y J	dry_PG	SO3	0.0000000000000000E+00	{~~}
557	START Y J	dry_PG	AR	0.3547417174159966E-02	{~~}
558	START M	PGcompressor	8	0.8320484335731876E-01	{~~}
559	START H	PGcompressor	8	-0.4466561290262733E+04	{~~}
560	START M	PGcompressor	9	-0.8320484335731876E-01	{~~}
561	START P		9	0.1038640799140263E+01	{~~}
562	START H	PGcompressor	9	-0.4453023621827175E+04	{~~}
563	START Q	PGcompressor	309	-0.2298774656334687E-01	{~~}
564	START W	PGcompressor	117	0.1149387328167349E+01	{~~}
565	START M	PGpreheat	11	0.1084136464468039E+00	{~~}
566	START P		11	0.1028640799140263E+01	{~~}
567	START H	PGpreheat	11	-0.6150749955252332E+04	{~~}
568	START M	PGpreheat	12	-0.1084136464468039E+00	{~~}
569	START P		12	0.1023640799140263E+01	{~~}
570	START H	PGpreheat	12	-0.6842868464426251E+04	{~~}
571	START M	PGpreheat	9	0.8320484335731876E-01	{~~}
572	START H	PGpreheat	9	-0.4453023621827175E+04	{~~}
573	START M	PGpreheat	10	-0.8320484335731876E-01	{~~}
574	START P		10	0.1033640799140263E+01	{~~}
575	START H	PGpreheat	10	-0.3551212040611453E+04	{~~}
576	START Q	PGpreheat	311	0.0000000000000000E+00	{~~}
577	START ZA	PGpreheat	1	0.7503509135286993E+02	{~~}
578	START M	aircompressor	31	0.7441554834157872E+00	{~~}
579	START P		31	0.1013000000000002E+01	{~~}
580	START H	aircompressor	31	-0.9883454496688249E+02	{~~}
581	START M	aircompressor	32	-0.7441554834157872E+00	{~~}
582	START P		32	0.1053640799140263E+01	{~~}
583	START H	aircompressor	32	-0.9336060792260105E+02	{~~}
584	START Q	aircompressor	312	-0.8313184219132176E-01	{~~}
585	START W	aircompressor	117	0.4156592109566154E+01	{~~}
586	START M	airpreheat2	35	0.7189466803263022E+00	{~~}
587	START P		35	0.1033640799140263E+01	{~~}
588	START H	airpreheat2	35	0.7462773132386449E+03	{~~}
589	START M	airpreheat2	36	-0.7189466803263022E+00	{~~}
590	START P		36	0.1023640799140263E+01	{~~}
591	START H	airpreheat2	36	0.1120243700978561E+03	{~~}
592	START M	airpreheat2	32	0.7441554834157872E+00	{~~}
593	START H	airpreheat2	32	-0.9336060792260105E+02	{~~}
594	START M	airpreheat2	34	-0.7441554834157872E+00	{~~}
595	START P		34	0.1043640799140263E+01	{~~}
596	START H	airpreheat2	34	0.5194065598541849E+03	{~~}
597	START Q	airpreheat2	314	0.0000000000000000E+00	{~~}
598	START ZA	airpreheat2	1	0.4559940479582562E+03	{~~}
599	START M	sofc	10	0.8320484335731876E-01	{~~}
600	START H	sofc	10	-0.3551212040611453E+04	{~~}
601	START M	sofc	34	0.7441554834157872E+00	{~~}
602	START H	sofc	34	0.5194065598541849E+03	{~~}
603	START M	sofc	11	-0.1084136464468039E+00	{~~}
604	START H	sofc	11	-0.6150749955252332E+04	{~~}
605	START M	sofc	35	-0.7189466803263022E+00	{~~}
606	START H	sofc	35	0.7462773132386449E+03	{~~}


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607 START E sofc 215 -0.2213328321455869E+03 {~~}
608 START Q sofc 315 0.0000000000000000E+00 {~~}
609 START ZA sofc 1 0.9348775972877994E+05 {~~}
610 START ZA sofc 2 0.8550154548146646E+05 {~~}
611 START ZA sofc 3 0.1170862073421318E+06 {~~}
612 START ZA sofc 4 0.2874558030874020E+06 {~~}
613 START ZA sofc 5 -0.4425649794871430E+06 {~~}
614 START ZA sofc 6 0.6890776990028493E+00 {~~}
615 START ZA sofc 7 0.8458535404752862E+00 {~~}
616 START ZA sofc 8 0.8500000000000001E+00 {~~}
617 START ZA sofc 9 0.4954299896595041E+00 {~~}
618 START ZA sofc 10 0.4097643685146286E+00 {~~}
619 START ZA sofc 11 0.9450055454564674E+00 {~~}
620 START ZA sofc 12 0.1080954241372454E+00 {~~}
621 START ZA sofc 13 0.7147434745365802E-02 {~~}
622 START ZA sofc 14 0.3042640018072583E-01 {~~}
623 START ZA sofc 15 0.7993362863931303E+00 {~~}
624 START ZA sofc 16 -0.8470853341704197E+05 {~~}
625 START ZA sofc 17 -0.1885369880714485E+06 {~~}
626 START ZA sofc 18 -0.1823577201067346E+06 {~~}
627 START ZA sofc 19 0.2821703056799879E+00 {~~}
628 START ZA sofc 20 0.2335762988681635E-01 {~~}
629 START ZA sofc 21 0.1013478073726874E+04 {~~}
630 START ZA sofc 22 0.3000000000000000E+03 {~~}
631 START ZA sofc 23 0.9500000000000001E+00 {~~}
632 START Y_J USED FUEL H2 0.3681288480481491E-01 {~~}
633 START Y_J USED FUEL CO 0.2592619821632520E-01 {~~}
634 START Y_J USED FUEL CO2 0.2785667382357346E+00 {~~}
635 START Y_J USED FUEL H2O-G 0.3654197752201502E+00 {~~}
636 START Y_J USED FUEL CH4 0.2245244540724863E-07 {~~}
637 START Y_J USED FUEL N2 0.2932743810705314E+00 {~~}
638 START Y_J USED FUEL O2 0.1825295746533185E+00 {~~}
639 START Y_J USED AIR N2 0.7972528602529357E+00 {~~}
640 START Y_J USED AIR CO2 0.3094525269451167E-03 {~~}
641 START Y_J USED AIR H2O-G 0.1041823507381893E-01 {~~}
642 START Y_J USED AIR AR 0.9489877492983592E-02 {~~}
643 START M burner 36 0.7189466803263022E+00 {~~}
644 START H burner 36 0.1120243700978561E+03 {~~}
645 START M burner 12 0.1084136464468039E+00 {~~}
646 START H burner 12 -0.6842868464426250E+04 {~~}
647 START M burner 41 -0.8273603267731059E+00 {~~}
648 START P 41 0.1023000000000002E+01 {~~}
649 START H burner 41 -0.7993140980860109E+03 {~~}
650 START Q burner 316 0.0000000000000000E+00 {~~}
651 START ZA burner 1 0.3738435658349209E+02 {~~}
652 START Y_J FLUE_GAS O2 0.1543733815328906E+00 {~~}
653 START Y_J FLUE_GAS N2 0.7324705619747473E+00 {~~}
654 START Y_J FLUE_GAS NO 0.0000000000000000E+00 {~~}
655 START Y_J FLUE_GAS CO2 0.4145268848345668E-01 {~~}
656 START Y_J FLUE_GAS H2O-G 0.6345676680902396E-01 {~~}
657 START Y_J FLUE_GAS SO2 0.0000000000000000E+00 {~~}
658 START Y_J FLUE_GAS NO2 0.0000000000000000E+00 {~~}
659 START Y_J FLUE_GAS AR 0.8246601199883187E-02 {~~}
660 START E el-motor 217 0.5585241513403690E+01 {~~}
661 START Q el-motor 317 -0.2792620756701864E+00 {~~}
662 START W el-motor 117 -0.5305979437733503E+01 {~~}
663 START M exhaustcooler 41 0.8273603267731059E+00 {~~}
664 START H exhaustcooler 41 -0.7993140980860109E+03 {~~}
665 START M exhaustcooler 44 -0.8273603267731059E+00 {~~}
666 START P 44 0.1013000000000002E+01 {~~}
667 START H exhaustcooler 44 -0.1002214102959687E+04 {~~}
668 START M exhaustcooler 85 0.8026077146914962E+00 {~~}
669 START P 85 0.1013000000000002E+01 {~~}
670 START H exhaustcooler 85 -0.1584524528596514E+05 {~~}
671 START M exhaustcooler 86 -0.8026077146914962E+00 {~~}
672 START P 86 0.1008000000000002E+01 {~~}
673 START H exhaustcooler 86 -0.1563608779686839E+05 {~~}
674 START Q exhaustcooler 319 0.0000000000000000E+00 {~~}
675 START ZA exhaustcooler 1 0.1678714143345494E+03 {~~}
676 C ~~~~~
677 C ~ End of generated initial guesses.
678 C ~~~~~

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end

DNA Output for SOFC scenario

1/6

1	Biomass gasification (Viking) + SOFC											
2	RUN NUMBER 1											
3												
4												
5												
6	ALGEBRAIC VARIABLES											
7	NO	TO	MEDIA	M	T	P	H	ENERGY	X	S	V	U
8	DE	COMPONENT		[kg/s]	[C]	[bar]	[kJ/kg]	[kJ/s]		[kJ/kg K]	[m3/kg]	[kJ/kg]
9	-----											
10	1	Dryer	Wood	0.04	15.00	-	-8621.6	4.991E+02	-	0.4612	-	-8621.6
11	64	Dryer	STEAM-HF	0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2
12	2	Dryer	DryWood	-0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1
13	61	Dryer	STEAM-HF	-0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1
14	301	Dryer	HEAT					0.000E+00				
15	2	Gasifier	DryWood	0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1
16	26	Gasifier	STEAM-HF	0.00	150.00	1.003	-13194.5		-	11.1292	1.9309	-13388.2
17	74	Gasifier	humid_air	0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7
18	3	Gasifier	raw_PG	-0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1
19	99	Gasifier	Ash	0.00	800.00	-	-4308.0		-	0.0000	-	-4308.0
20	302	Gasifier	HEAT					0.000E+00				
21	3	airpreheat	raw_PG	0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1
22	4	airpreheat	raw_PG	-0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7
23	72	airpreheat	STANDARD_AIR	0.04	15.00	1.008	-98.8		-	6.8668	0.8237	-181.9
24	73	airpreheat	STANDARD_AIR	-0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1
25	303	airpreheat	HEAT					0.000E+00				
26	4	steamheater	raw_PG	0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7
27	5	steamheater	raw_PG	-0.09	259.48	0.988	-4375.3		-	9.7468	2.0710	-4579.9
28	63	steamheater	STEAM-HF	0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
29	64	steamheater	STEAM-HF	-0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2
30	304	steamheater	HEAT					0.000E+00				
31	61	steamblower	STEAM-HF	0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1
32	62	steamblower	STEAM-HF	-0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
33	305	steamblower	HEAT					-1.409E-02				
34	105	steamblower	MECH_POWER					7.044E-01				
35	62	split1	STEAM-HF	0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
36	63	split1	STEAM-HF	-0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
37	69	split1	STEAM-HF	-0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
38	73	mix1	STANDARD_AIR	0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1
39	69	mix1	STEAM-HF	0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6
40	74	mix1	humid_air	-0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7
41	5	gascooler	raw_PG	0.09	259.48	0.988	-4375.3		-	9.7468	2.0710	-4579.9
42	6	gascooler	cold_PG	-0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1
43	98	gascooler	STEAM-HF	0.00	90.00	0.983	-15594.1		-	4.7085	0.0010	-15594.2
44	81	gascooler	STEAM-HF	0.10	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3
45	82	gascooler	STEAM-HF	-0.10	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
46	306	gascooler	HEAT					0.000E+00				
47	6	gasclean	cold_PG	0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1
48	7	gasclean	clean_PG	-0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4
49	97	gasclean	impurities	0.00	90.00	0.978	-535.6		-	6.2438	0.9059	-624.2
50	307	gasclean	HEAT					0.000E+00				
51	7	condenser	clean_PG	0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4
52	8	condenser	dry_PG	-0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1
53	96	condenser	STEAM-HF	0.00	50.01	0.973	-15761.7		-	4.2198	0.0010	-15761.7
54	83	condenser	STEAM-HF	0.05	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3
55	84	condenser	STEAM-HF	-0.05	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
56	308	condenser	HEAT					0.000E+00				
57	8	PGcompressor	dry_PG	0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1

DNA Output for SOFC scenario

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58	9	PGcompressor	dry_PG		-0.08	59.55	1.039	-4453.0		-	8.9761	1.2244	-4580.2
59	309	PGcompressor	HEAT					-2.299E-02					
60	117	PGcompressor	MECH_POWER					1.149E+00					
61	11	PGpreheat	USED_FUEL		0.11	800.00	1.029	-6150.7		-	9.0717	3.1135	-6471.0
62	12	PGpreheat	USED_FUEL		-0.11	316.78	1.024	-6842.9		-	8.2220	1.7199	-7018.9
63	9	PGpreheat	dry_PG		0.08	59.55	1.039	-4453.0		-	8.9761	1.2244	-4580.2
64	10	PGpreheat	dry_PG		-0.08	650.00	1.034	-3551.2		-	10.5180	3.4139	-3904.1
65	311	PGpreheat	HEAT					0.000E+00					
66	31	aircompressor	STANDARD_AIR		0.74	15.00	1.013	-98.8		-	6.8653	0.8196	-181.9
67	32	aircompressor	STANDARD_AIR		-0.74	20.42	1.054	-93.4		-	6.8728	0.8028	-178.0
68	312	aircompressor	HEAT					-8.313E-02					
69	117	aircompressor	MECH_POWER					4.157E+00					
70	35	airpreheat2	USED_AIR		0.72	800.00	1.034	746.3		-	8.2601	3.0019	436.0
71	36	airpreheat2	USED_AIR		-0.72	224.33	1.024	112.0		-	7.4222	1.4052	-31.8
72	32	airpreheat2	STANDARD_AIR		0.74	20.42	1.054	-93.4		-	6.8728	0.8028	-178.0
73	34	airpreheat2	STANDARD_AIR		-0.74	600.00	1.044	519.4		-	8.0168	2.4107	267.8
74	314	airpreheat2	HEAT					0.000E+00					
75	10	sofc	dry_PG		0.08	650.00	1.034	-3551.2		-	10.5180	3.4139	-3904.1
76	34	sofc	STANDARD_AIR		0.74	600.00	1.044	519.4		-	8.0168	2.4107	267.8
77	11	sofc	USED_FUEL		-0.11	800.00	1.029	-6150.7		-	9.0717	3.1135	-6471.0
78	35	sofc	USED_AIR		-0.72	800.00	1.034	746.3		-	8.2601	3.0019	436.0
79	215	sofc	ELECT_POWER					-2.213E+02					
80	315	sofc	HEAT					0.000E+00					
81	217	el-motor	ELECT_POWER					5.585E+00					
82	317	el-motor	HEAT					-2.793E-01					
83	117	el-motor	MECH_POWER					-5.306E+00					
84	36	burner	USED_AIR		0.72	224.33	1.024	112.0		-	7.4222	1.4052	-31.8
85	12	burner	USED_FUEL		0.11	316.78	1.024	-6842.9		-	8.2220	1.7199	-7018.9
86	41	burner	FLUE_GAS		-0.83	310.20	1.023	-799.3		-	7.7021	1.6487	-968.0
87	316	burner	HEAT					0.000E+00					
88	41	exhaustcooler	FLUE_GAS		0.83	310.20	1.023	-799.3		-	7.7021	1.6487	-968.0
89	44	exhaustcooler	FLUE_GAS		-0.83	120.02	1.013	-1002.2		-	7.2845	1.1222	-1115.9
90	85	exhaustcooler	STEAM-HF		0.80	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3
91	86	exhaustcooler	STEAM-HF		-0.80	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
92	319	exhaustcooler	HEAT					0.000E+00					
93	-----												
94													
95													
96	EXERGY												
97													
98	NO	TO	MEDIA		E_PH	E_CH	E	EX_PH	EX_CH	EX			
99	DE	COMPONENT			[kJ/kg]	[kJ/kg]	[kJ/kg]	[kJ/s]	[kJ/s]	[kJ/s]			
100	-----												
101	1	Dryer	Wood		0.00	13311.33	13311.33	0.00	572.39	572.39			
102	64	Dryer	STEAM-HF		660.71	-	660.71	132.17	-	132.17			
103	2	Dryer	DryWood		-54.56	18651.57	18597.01	1.67	-572.39	-570.71			
104	61	Dryer	STEAM-HF		583.11	-	583.11	-123.83	-	-123.83			
105	301	Dryer	HEAT		-	-	-	0.00	0.00	0.00			
106	2	Gasifier	DryWood		-54.56	18651.57	18597.01	-1.67	572.39	570.71			
107	26	Gasifier	STEAM-HF		584.41	-	584.41	0.00	-	0.00			
108	74	Gasifier	humid_air		310.33	66.40	376.73	17.02	3.64	20.66			
109	3	Gasifier	raw_PG		644.70	5438.32	6083.02	-54.98	-463.75	-518.73			
110	99	Gasifier	Ash		785.00	-	785.00	-0.21	-	-0.21			
111	302	Gasifier	HEAT		-	-	-	0.00	0.00	0.00			
112	3	airpreheat	raw_PG		644.70	5438.32	6083.02	54.98	463.75	518.73			
113	4	airpreheat	raw_PG		358.65	5438.32	5796.96	-30.58	-463.75	-494.34			
114	72	airpreheat	STANDARD_AIR		0.66	3.73	4.39	0.03	0.16	0.19			

DNA Output for SOFC scenario

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115	73	airpreheat	STANDARD_AIR	427.84	3.73	431.57	-18.20	-0.16	-18.36
116	303	airpreheat	HEAT	-	-	-	0.00	0.00	0.00
117	4	steamheater	raw_PG	358.65	5438.32	5796.96	30.58	463.75	494.34
118	5	steamheater	raw_PG	97.80	5438.32	5536.12	-8.34	-463.75	-472.09
119	63	steamheater	STEAM-HF	585.47	-	585.47	117.12	-	117.12
120	64	steamheater	STEAM-HF	660.71	-	660.71	-132.17	-	-132.17
121	304	steamheater	HEAT	-	-	-	0.00	0.00	0.00
122	61	steamblower	STEAM-HF	583.11	-	583.11	123.83	-	123.83
123	62	steamblower	STEAM-HF	585.47	-	585.47	-124.33	-	-124.33
124	305	steamblower	HEAT	-	-	-	0.00	0.00	0.00
125	105	steamblower	MECH_POWER	-	-	-	0.70	0.00	0.70
126	62	split1	STEAM-HF	585.47	-	585.47	124.33	-	124.33
127	63	split1	STEAM-HF	585.47	-	585.47	-117.12	-	-117.12
128	69	split1	STEAM-HF	585.47	-	585.47	-7.21	-	-7.21
129	73	mix1	STANDARD_AIR	427.84	3.73	431.57	18.20	0.16	18.36
130	69	mix1	STEAM-HF	585.47	-	585.47	7.21	-	7.21
131	74	mix1	humid_air	310.33	66.40	376.73	-17.02	-3.64	-20.66
132	5	gascooler	raw_PG	97.80	5438.32	5536.12	8.34	463.75	472.09
133	6	gascooler	cold_PG	10.04	5438.32	5448.36	-0.86	-463.75	-464.61
134	98	gascooler	STEAM-HF	34.93	-	34.93	0.00	-	0.00
135	81	gascooler	STEAM-HF	1.49	-	1.49	0.15	-	0.15
136	82	gascooler	STEAM-HF	26.73	-	26.73	-2.72	-	-2.72
137	306	gascooler	HEAT	-	-	-	0.00	0.00	0.00
138	6	gasclean	cold_PG	10.04	5438.32	5448.36	0.86	463.75	464.61
139	7	gasclean	clean_PG	9.49	5437.03	5446.52	-0.81	-463.61	-464.42
140	97	gasclean	impurities	6.93	23829.09	23836.02	0.00	-0.15	-0.15
141	307	gasclean	HEAT	-	-	-	0.00	0.00	0.00
142	7	condenser	clean_PG	9.49	5437.03	5446.52	0.81	463.61	464.42
143	8	condenser	dry_PG	-0.23	5566.16	5565.93	0.02	-463.13	-463.11
144	96	condenser	STEAM-HF	8.19	-	8.19	-0.02	-	-0.02
145	83	condenser	STEAM-HF	1.49	-	1.49	0.07	-	0.07
146	84	condenser	STEAM-HF	26.73	-	26.73	-1.25	-	-1.25
147	308	condenser	HEAT	-	-	-	0.00	0.00	0.00
148	8	PGcompressor	dry_PG	-0.23	5566.16	5565.93	-0.02	463.13	463.11
149	9	PGcompressor	dry_PG	8.60	5566.16	5574.75	-0.72	-463.13	-463.85
150	309	PGcompressor	HEAT	-	-	-	0.00	0.00	0.00
151	117	PGcompressor	MECH_POWER	-	-	-	1.15	0.00	1.15
152	11	PGpreheat	USED_FUEL	570.75	787.09	1357.84	61.88	85.33	147.21
153	12	PGpreheat	USED_FUEL	123.47	787.09	910.56	-13.39	-85.33	-98.72
154	9	PGpreheat	dry_PG	8.60	5566.16	5574.75	0.72	463.13	463.85
155	10	PGpreheat	dry_PG	466.12	5566.16	6032.28	-38.78	-463.13	-501.92
156	311	PGpreheat	HEAT	-	-	-	0.00	0.00	0.00
157	31	aircompressor	STANDARD_AIR	1.07	3.73	4.81	0.80	2.78	3.58
158	32	aircompressor	STANDARD_AIR	4.39	3.73	8.12	-3.27	-2.78	-6.04
159	312	aircompressor	HEAT	-	-	-	0.00	0.00	0.00
160	117	aircompressor	MECH_POWER	-	-	-	4.16	0.00	4.16
161	35	airpreheat2	USED_AIR	448.07	3.78	451.85	322.14	2.72	324.86
162	36	airpreheat2	USED_AIR	55.27	3.78	59.05	-39.73	-2.72	-42.45
163	32	airpreheat2	STANDARD_AIR	4.39	3.73	8.12	3.27	2.78	6.04
164	34	airpreheat2	STANDARD_AIR	287.52	3.73	291.25	-213.96	-2.78	-216.74
165	314	airpreheat2	HEAT	-	-	-	0.00	0.00	0.00
166	10	sofc	dry_PG	466.12	5566.16	6032.28	38.78	463.13	501.92
167	34	sofc	STANDARD_AIR	287.52	3.73	291.25	213.96	2.78	216.74
168	11	sofc	USED_FUEL	570.75	787.09	1357.84	-61.88	-85.33	-147.21
169	35	sofc	USED_AIR	448.07	3.78	451.85	-322.14	-2.72	-324.86

DNA Output for SOFC scenario

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170	215	sofc	ELECT_POWER		-		-		-		-221.33		0.00		-221.33			
171	315	sofc	HEAT		-		-		-		0.00		0.00		0.00			
172	217	el-motor	ELECT_POWER		-		-		-		5.59		0.00		5.59			
173	317	el-motor	HEAT		-		-		-		0.00		0.00		0.00			
174	117	el-motor	MECH_POWER		-		-		-		-5.31		0.00		-5.31			
175	36	burner	USEDAIR		55.27		3.78		59.05		39.73		2.72		42.45			
176	12	burner	USEDFUEL		123.47		787.09		910.56		13.39		85.33		98.72			
177	41	burner	FLUE_GAS		99.77		20.90		120.66		-82.54		-17.29		-99.83			
178	316	burner	HEAT		-		-		-		0.00		0.00		0.00			
179	41	exhaustcooler	FLUE_GAS		99.77		20.90		120.66		82.54		17.29		99.83			
180	44	exhaustcooler	FLUE_GAS		17.18		20.90		38.08		-14.21		-17.29		-31.50			
181	85	exhaustcooler	STEAM-HF		1.49		-		1.49		1.20		-		1.20			
182	86	exhaustcooler	STEAM-HF		26.73		-		26.73		-21.45		-		-21.45			
183	319	exhaustcooler	HEAT		-		-		-		0.00		0.00		0.00			
184	-----																	
185																		
186	ELEC. POWER PRODUCTION =		221.3328 kW															
187	TOTAL POWER CONSUMPTION =		6.2896 kW															
188	NET POWER PRODUCTION =		215.0432 kW															
189	FUEL CONSUMPTION (LHV) =		499.1161 kJ/s															
190	FUEL CONSUMPTION (HHV) =		572.3872 kJ/s															
191	THERMAL EFFICIENCY (LHV)=		0.4308															
192	THERMAL EFFICIENCY (HHV)=		0.3757															
193																		
194	MAXIMUM RELATIVE ERROR =		8.8267E-13															
195	COMPUTER ACCURACY =		1.0842E-19															
196																		
197																		
198																		
199	IDEAL GAS COMPOSITION (MOLAR BASE):																	
200																		
201		humid_air	raw_PG		STANDARD_AIR	cold_PG		clean_PG										
202	-----																	
203	HYDROGEN		0.0000E+00		0.2538E+00		0.0000E+00		0.2538E+00		0.2538E+00							
204	OXYGEN		0.1418E+00		0.0000E+00		0.2075E+00		0.0000E+00		0.0000E+00							
205	NITROGEN		0.5281E+00		0.2897E+00		0.7729E+00		0.2897E+00		0.2897E+00							
206	CARBON MONOXIDE		0.0000E+00		0.1762E+00		0.0000E+00		0.1762E+00		0.1762E+00							
207	CARBON DIOXIDE		0.2050E-03		0.1144E+00		0.3000E-03		0.1144E+00		0.1144E+00							
208	WATER (I.G.)		0.3236E+00		0.1523E+00		0.1010E-01		0.1523E+00		0.1523E+00							
209	HYDROGEN SULFIDE		0.0000E+00		0.4616E-04		0.0000E+00		0.4616E-04		0.0000E+00							
210	METHANE		0.0000E+00		0.1011E-01		0.0000E+00		0.1011E-01		0.1011E-01							
211	ARGON		0.6286E-02		0.3444E-02		0.9200E-02		0.3444E-02		0.3444E-02							
212	-----																	
213	MEAN MOLE MASS		0.2542E+02		0.2164E+02		0.2885E+02		0.2164E+02		0.2164E+02							
214	NET CALORI VALUE		0.0000E+00		0.5516E+04		0.0000E+00		0.5516E+04		0.5515E+04							
215	GRS CALORI VALUE		0.0000E+00		0.1148E+05		0.0000E+00		0.1148E+05		0.1148E+05							
216	-----																	
217																		
218	IDEAL GAS COMPOSITION (MOLAR BASE):																	
219																		
220		impurities	dry_PG		USEDFUEL	USEDAIR		FLUE_GAS										
221	-----																	
222	HYDROGEN		0.0000E+00		0.2614E+00		0.3681E-01		0.0000E+00		0.0000E+00							
223	OXYGEN		0.0000E+00		0.0000E+00		0.0000E+00		0.1825E+00		0.1544E+00							
224	NITROGEN		0.0000E+00		0.2983E+00		0.2933E+00		0.7973E+00		0.7325E+00							
225	CARBON MONOXIDE		0.0000E+00		0.1815E+00		0.2593E-01		0.0000E+00		0.0000E+00							
226	CARBON DIOXIDE		0.0000E+00		0.1179E+00		0.2786E+00		0.3095E-03		0.4145E-01							
227	WATER (I.G.)		0.0000E+00		0.1269E+00		0.3654E+00		0.1042E-01		0.6346E-01							
228	HYDROGEN SULFIDE		0.1000E+01		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00							

DNA Output for SOFC scenario

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229 METHANE          | 0.0000E+00 | 0.1042E-01 | 0.2245E-07 | 0.0000E+00 | 0.0000E+00 |
230 ARGON            | 0.0000E+00 | 0.3547E-02 | 0.0000E+00 | 0.9490E-02 | 0.8247E-02 |
231 -----
232 MEAN MOLE MASS| 0.3408E+02 | 0.2175E+02 | 0.2786E+02 | 0.2875E+02 | 0.2876E+02 |
233 NET CALORI VALUE| 0.1521E+05 | 0.5652E+04 | 0.5829E+03 | 0.0000E+00 | 0.0000E+00 |
234 GRS CALORI VALUE| 0.1650E+05 | 0.1172E+05 | 0.2279E+04 | 0.0000E+00 | 0.0000E+00 |
235 -----
236
237 NON-IDEAL FLUID AND SOLID COMPOSITION (MASS BASE):
238
239          |Wood          |DryWood      |Ash          |
240 -----
241 HYDROGEN      | 0.4204E-01 | 0.5890E-01 | 0.0000E+00 |
242 OXYGEN         | 0.2976E+00 | 0.4171E+00 | 0.0000E+00 |
243 NITROGEN       | 0.1153E-02 | 0.1615E-02 | 0.0000E+00 |
244 CARBON (SOLID) | 0.3309E+00 | 0.4636E+00 | 0.0000E+00 |
245 SULFUR (SOLID) | 0.1356E-03 | 0.1900E-03 | 0.0000E+00 |
246 WATER (LIQUID) | 0.3220E+00 | 0.5000E-01 | 0.0000E+00 |
247 ASHES         | 0.6170E-02 | 0.8645E-02 | 0.1000E+01 |
248 -----
249 MEAN MOLE MASS| 0.1321E+02 | 0.1193E+02 | 0.7600E+02 |
250 NET CALORI VALUE| 0.1161E+05 | 0.1724E+05 | 0.0000E+00 |
251 GRS CALORI VALUE| 0.1331E+05 | 0.1865E+05 | 0.0000E+00 |
252 -----
253
254 MEDIUM 97 : WATER FOR GAS APP
255 MEDIUM 300 : HEAT
256 MEDIUM 301 : PRODUCT HEAT
257
258
259 NUMBER OF CLOSED INTERNAL LOOPS IN THE SYSTEM:    0
260
261
262
263
264
265 SOLUTION FOR THE INDEPENDENT ALGEBRAIC VARIABLES :
266
267
268 VARIABLE NO | COMPONENT      | NAME          | VALUE      |
269 -----
270      1      |Gasifier        |MULTIPLIER H| 0.8501E+05 |
271      2      |Gasifier        |MULTIPLIER C| 0.4364E+05 |
272      3      |Gasifier        |MULTIPLIER N| 0.1173E+06 |
273      4      |Gasifier        |MULTIPLIER O| 0.3125E+06 |
274      5      |Gasifier        |MULTIPLIER S| 0.1828E+06 |
275      6      |Gasifier        |MULTIPL Ar   | 0.2292E+06 |
276      7      |Gasifier        |GIBBS ENERGY| -.3280E+06 |
277      1      |airpreheat      |Transferred  | 0.3503E+02 |
278      1      |steamheater      |Transferred  | 0.3894E+02 |
279      1      |PGpreheat       |Transferred  | 0.7504E+02 |
280      1      |airpreheat2     |Transferred  | 0.4560E+03 |
281      1      |sofc            |MULTIPLIER H| 0.9349E+05 |
282      2      |sofc            |MULTIPLIER C| 0.8550E+05 |
283      3      |sofc            |MULTIPLIER N| 0.1171E+06 |
284      4      |sofc            |MULTIPLIER O| 0.2875E+06 |
285      5      |sofc            |GIBBS ENERGY| -.4426E+06 |
286      6      |sofc            |ETAMAX       | 0.6891E+00 |
287      7      |sofc            |ETASYS       | 0.8459E+00 |
288      8      |sofc            |UF           | 0.8500E+00 |
289      9      |sofc            |ETATOT       | 0.4954E+00 |
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DNA Output for SOFC scenario

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290      10      |sofc      |STCR      | 0.4098E+00 |
291      11      |sofc      |E_nernst   | 0.9450E+00 |
292      12      |sofc      |V_act      | 0.1081E+00 |
293      13      |sofc      |V_ohm      | 0.7147E-02 |
294      14      |sofc      |V_conc     | 0.3043E-01 |
295      15      |sofc      |V_cell     | 0.7993E+00 |
296      16      |sofc      |GMAX       | -.8471E+05 |
297      17      |sofc      |G(T)       | -.1885E+06 |
298      18      |sofc      |G(p,T)     | -.1824E+06 |
299      19      |sofc      |p_H2eq     | 0.2822E+00 |
300      20      |sofc      |R_e        | 0.2336E-01 |
301      21      |sofc      |Area [cm^2]| 0.1013E+04 |
302      22      |sofc      |i_load     | 0.3000E+03 |
303      23      |sofc      |eta_DCAC   | 0.9500E+00 |
304      1       |burner     |Lambda     | 0.3738E+02 |
305      1       |exhaustcooler |Transferred | 0.1679E+03 |
306 -----
307
308 =====
309 #####
end
```

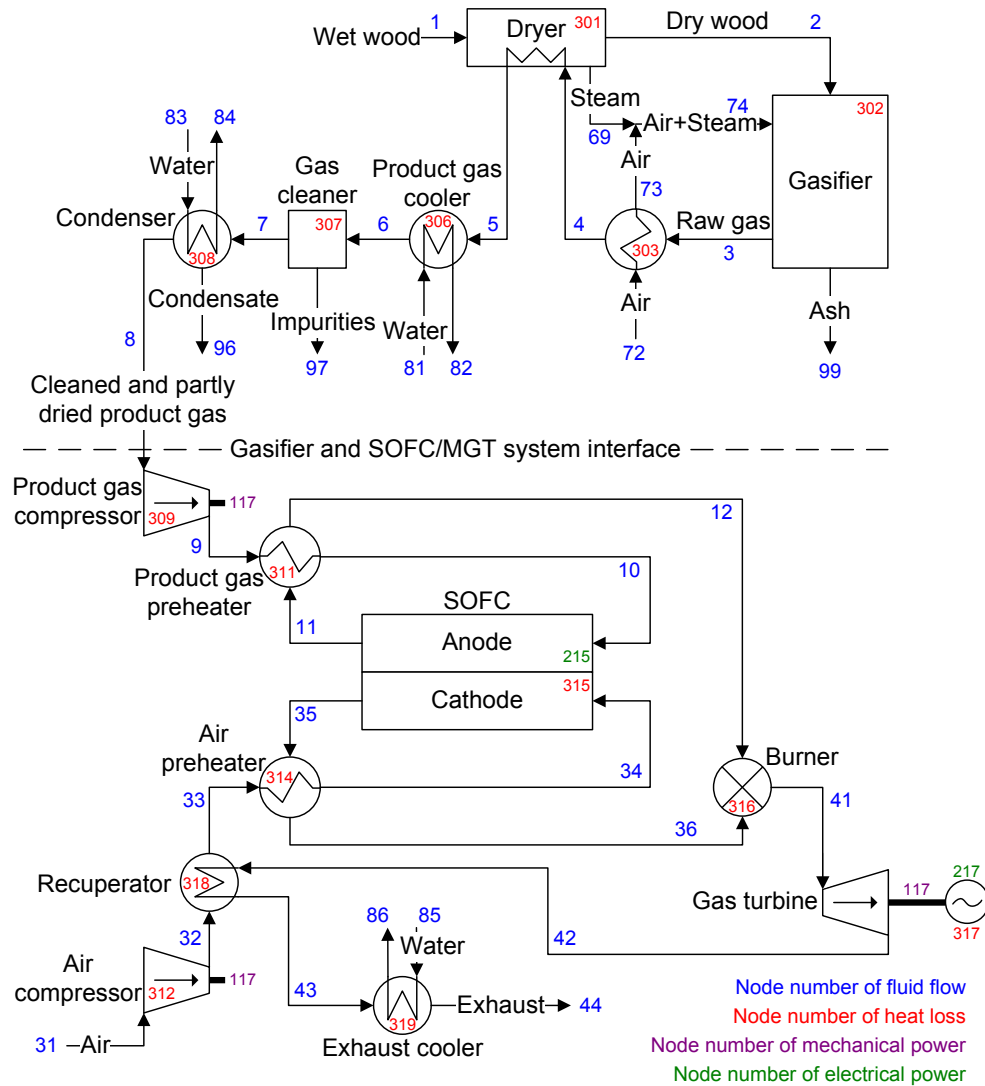
Appendix E SOFC-MGT PLANT MODEL LISTING

Included in this Appendix are:

- Flow sheet of SOFC-MGT scenario with node numbers (1 page)
- DNA Input for SOFC-MGT scenario (10 pages)
- DNA Output for SOFC-MGT scenario (7 pages)

The input and output data only represent one simulation using the reference conditions.

Flow sheet of SOFC-MGT scenario with node numbers



DNA Input for SOFC-MGT scenario

1/10

```
1 title Biomass gasification (Viking) + SOFC/MGT incl. recuperation
2 C Wood is dried and gasified. The gasification is atmospheric,
3 C based on air, and almost reaches equilibrium. The produced
4 C product gas (PG) composition and the cold gas efficiency is
5 C similar to that from the Viking gasifier.
6 C Power and heat production by a hybrid SOFC/MGT system.
7
8
9 C #####
10 C #####
11 C #####
12 C -----GASIFIER PART-----
13 C #####
14 C #####
15 C #####
16
17 C ##Media##
18 media 1 Wood 2 DryWood
19 media 73 STANDARD_AIR 3 raw_PG 99 Ash
20
21 C ##Fuel composition##
22 solid Wood C 0.488 H .062 O .439 S .0002 N 0.0017 ASH .0091
23 + LHV 18280 CP 1.35 MOI .322
24 C [Ahrenfeldt, J. et al., Energy & Fuels 2006, 20, 2672-2680] without Cl.
25
26
27
28 C #####
29 C -----DRYER-----
30 C #####
31 struc Dryer DRYER_03 1 64 2 61 301 0.05 0.005
32
33 C Fuel input (plant size):
34 addco m Dryer 1 0.043
35
36 addco t Dryer 1 15 p 1 1.013
37 addco p 2 1.008 t Dryer 2 150
38 addco q Dryer 301 0
39
40
41
42 C #####
43 C -----GASIFIER-----
44 C #####
45 struc Gasifier GASIFI_3 8 2 26 74 3 99 302 1 3 4 6 7 9 11 36 /
46 0.998 800 0.005 0 1.0 0.01
47 C Variable constitution parameter: Number of calculated gas components 8
48 C Nodes: Inlet fuel 2; inlet water 26; inlet air 74; outlet PG 3,
49 C outlet ash 99, heat loss 302
50 C Integer Parameters: Calculated gas compounds H2 (1), N2 (3), CO (4),
51 C CO2 (6), H2O (7), H2S (9), CH4 (11), Ar (36)
52 C Real parameter: Pressure 1 bar, Eq. temperature 800 degC, Pressure loss 0,
53 C Water-to-fuel ratio 0, carbon conversion factor 1,
54 C non-equilibrium methane 0.01.
55
56 addco t Gasifier 3 800
57 addco t Gasifier 26 150
58 addco p 99 1.013
59 addco q Gasifier 302 0
60
61
62
63 C #####
64 C -----GASIFIER AIR PREHEATER-----
65 C #####
66 struc airpreheat heatex_2 3 4 72 73 303 20 0.005 0.005
67 addco t airpreheat 72 15
68 addco q airpreheat 303 0
69
70
71
72 C #####
73 C -----STEAM HEATER-----
74 C #####
75 struc steamheater heatex_1 4 5 63 64 304 0.005 0.005
76
```


DNA Input for SOFC–MGT scenario

2/10

```
77 media 63 STEAM-HF
78
79 addco t steamheater 64 250
80 addco q steamheater 304 0
81
82
83
84 C #####
85 C -----STEAM BLOWER-----
86 C #####
87 struc steamblower COMPRE_1 61 62 305 105 0.6 0.98
88
89
90
91 C #####
92 C -----SPLITTER-----
93 C #####
94 struc split1 SPLITTER 62 63 69
95
96
97
98 C #####
99 C -----MIXER-----
100 C #####
101 struc mix1 MIXER_02 73 69 74
102
103 media 74 humid_air
104
105
106
107 C #####
108 C -----GAS COOLER-----
109 C #####
110 struc gascooler GASCOOL1 5 6 98 81 82 306 0.005 0.005
111
112 media 81 STEAM-HF 6 cold_PG
113
114 addco t gascooler 6 90
115 addco t gascooler 81 30 p 81 1.013
116 addco t gascooler 82 80
117 addco q gascooler 306 0
118
119
120
121 C #####
122 C -----GAS CLEANING-----
123 C #####
124 struc gasclean GASCLE_1 6 7 97 307 0.0049
125 C Pressure loss is taken from paper about Viking
126
127 media 7 clean_PG 97 impurities
128
129 addco q gasclean 307 0
130
131
132
133 C #####
134 C -----CONDENSER-----
135 C #####
136 struc condenser GASCOOL1 7 8 96 83 84 308 0.005 0.005
137
138 media 83 STEAM-HF 8 dry_PG
139
140 addco t condenser 8 50
141 addco t condenser 83 30 p 83 1.013
142 addco t condenser 84 80
143 addco q condenser 308 0
144
145
146
147 C #####
148 C #####
149 C #####
150 C -----SOFC/MGT PART-----
151 C #####
152 C #####
```

DNA Input for SOFC-MGT scenario

3/10

```
153 C #####
154
155 media 11 USED_FUEL 35 USED_AIR
156
157
158
159 C #####
160 C -----PRODUCT GAS COMPRESSOR-----
161 C #####
162 struc PGcompressor compre_1 8 9 309 117 0.75 0.98
163 C Isentropic efficiency from L. Fryda et al. (2008)
164
165
166
167 C #####
168 C -----PRODUCT GAS PREHEATING-----
169 C #####
170 struc PGpreheat heatex_2 11 12 9 10 311 150 0.005 0.005
171 addco q PGpreheat 311 0
172
173
174
175 C #####
176 C -----AIR COMPRESSOR-----
177 C #####
178 struc aircompressor compre_1 31 32 312 117 0.75 0.98
179 C Isentropic efficiency from L. Fryda et al. (2008)
180
181 media 31 STANDARD_AIR
182
183 addco p 31 1.013 t aircompressor 31 15
184
185
186
187 C #####
188 C -----RECUPERATOR-----
189 C #####
190 struc recuperator heatex_4 42 43 32 33 318 0.85 0.01 0.01
191 addco q recuperator 318 0
192
193
194
195 C #####
196 C -----SOFC AIR PREHEATING-----
197 C #####
198 struc airpreheat2 heatex_2 35 36 33 34 314 200 0.01 0.01
199 addco q airpreheat2 314 0
200
201
202
203 C #####
204 C -----SOFC-----
205 C #####
206 struc sofc sofcq0d_CBM /
207     {fuel and air inlets} 10 34 /
208     {fuel and air outlets} 11 35 /
209     {nodes for power and heat loss} 215 315 /
210     {parameters: utilization, temperature} 0.85 800 /
211     {pressure loss} 0.005 0.010 /
212     {temperature difference between anode and cathode outlet} 0 /
213     {current density [mA/cm^2]} 300 /
214     {DC to AC conversion efficiency [-]} 0.95
215
216 addco q sofc 315 0
217
218 C SOFC OPERATING PRESSURE:
219 addco p 10 2.5
220
221
222
223 C #####
224 C -----BURNER-----
225 C #####
226 struc burner GASBUR_3 36 12 41 316 0.999374
227
228 media 41 FLUE_GAS
```

```

229
230 addco q burner 316 0
231
232
233
234 C #####
235 C -----GAS TURBINE-----
236 C #####
237 struc GT turbin_1 41 42 117 0.84
238 C Isentropic efficiency from L. Fryda et al. (2008)
239
240
241
242 C #####
243 C -----GENERATOR-----
244 C #####
245 struc generator sim_gene 217 317 117 0.95
246
247
248
249 C #####
250 C -----EXHAUST COOLING-----
251 C #####
252 struc exhaustcooler heatex_2 43 44 85 86 319 90 0.010 0.005
253
254 media 85 STEAM-HF
255
256 addco p 44 1.013
257 addco p 85 1.013 t exhaustcooler 85 30
258 addco t exhaustcooler 86 80
259 addco q exhaustcooler 319 0
260
261
262
263 C Reference conditions for exergy
264 xergy p 1 t 15
265
266
267
268
269
270 C ~~~~~
271 C ~~ Start of list of generated initial guesses.
272 C ~~ The values are the results of the latest simulation.
273 C ~~~~~
274
275
276
277
278
279
280
281
282
283
284
285
286
287
288
289
290
291
292
293
294
295
296
297
298
299
300
301
302

```

START M	Dryer	1	0.430000000000000013E-01	{~~}
START P		1	0.101300000000000003E+01	{~~}
START H	Dryer	1	-0.8621618755529560E+04	{~~}
START M	Dryer	64	0.2000459030657081E+00	{~~}
START P		64	0.998000000000000029E+00	{~~}
START H	Dryer	64	-0.1299653551379776E+05	{~~}
START M	Dryer	2	-0.3068842105263166E-01	{~~}
START P		2	0.100800000000000003E+01	{~~}
START H	Dryer	2	-0.5497059220211016E+04	{~~}
START M	Dryer	61	-0.2123574820130765E+00	{~~}
START P		61	0.993000000000000029E+00	{~~}
START H	Dryer	61	-0.1319443607829823E+05	{~~}
START Q	Dryer	301	0.000000000000000000E+00	{~~}
START X_J	DryWood	H2	0.589000000000000016E-01	{~~}
START X_J	DryWood	O2	0.417050000000000013E+00	{~~}
START X_J	DryWood	N2	0.161500000000000005E-02	{~~}
START X_J	DryWood	CO	0.000000000000000000E+00	{~~}
START X_J	DryWood	NO	0.000000000000000000E+00	{~~}
START X_J	DryWood	CO2	0.000000000000000000E+00	{~~}
START X_J	DryWood	H2O-L	0.500000000000000014E-01	{~~}
START X_J	DryWood	NH3	0.000000000000000000E+00	{~~}
START X_J	DryWood	H2S	0.000000000000000000E+00	{~~}
START X_J	DryWood	SO2	0.000000000000000000E+00	{~~}
START X_J	DryWood	CH4	0.000000000000000000E+00	{~~}
START X_J	DryWood	C2H6	0.000000000000000000E+00	{~~}
START X_J	DryWood	C3H8	0.000000000000000000E+00	{~~}
START X_J	DryWood	C4H10-N	0.000000000000000000E+00	{~~}
START X_J	DryWood	C4H10-I	0.000000000000000000E+00	{~~}
START X_J	DryWood	C5H12	0.000000000000000000E+00	{~~}

303	START X_J	DryWood	C6H14	0.0000000000000000E+00	{~~}
304	START X_J	DryWood	C7H16	0.0000000000000000E+00	{~~}
305	START X_J	DryWood	C8H18	0.0000000000000000E+00	{~~}
306	START X_J	DryWood	C2H4	0.0000000000000000E+00	{~~}
307	START X_J	DryWood	C3H6	0.0000000000000000E+00	{~~}
308	START X_J	DryWood	C5H10	0.0000000000000000E+00	{~~}
309	START X_J	DryWood	C6H12-1	0.0000000000000000E+00	{~~}
310	START X_J	DryWood	C7H14	0.0000000000000000E+00	{~~}
311	START X_J	DryWood	C2H2	0.0000000000000000E+00	{~~}
312	START X_J	DryWood	C6H6	0.0000000000000000E+00	{~~}
313	START X_J	DryWood	C6H12-C	0.0000000000000000E+00	{~~}
314	START X_J	DryWood	C	0.4636000000000001E+00	{~~}
315	START X_J	DryWood	S	0.1900000000000006E-03	{~~}
316	START X_J	DryWood	NO2	0.0000000000000000E+00	{~~}
317	START X_J	DryWood	HCN	0.0000000000000000E+00	{~~}
318	START X_J	DryWood	COS	0.0000000000000000E+00	{~~}
319	START X_J	DryWood	N2O	0.0000000000000000E+00	{~~}
320	START X_J	DryWood	NO3	0.0000000000000000E+00	{~~}
321	START X_J	DryWood	SO3	0.0000000000000000E+00	{~~}
322	START X_J	DryWood	AR	0.0000000000000000E+00	{~~}
323	START X_J	DryWood	ASH	0.8645000000000028E-02	{~~}
324	START X_J	DryWood	TAR	0.0000000000000000E+00	{~~}
325	START M	Gasifier	2	0.3068842105263166E-01	{~~}
326	START H	Gasifier	2	-0.5497059220211016E+04	{~~}
327	START M	Gasifier	26	0.0000000000000000E+00	{~~}
328	START P		26	0.1003000000000003E+01	{~~}
329	START H	Gasifier	26	-0.1319450918722709E+05	{~~}
330	START M	Gasifier	74	0.5485206982616307E-01	{~~}
331	START P		74	0.1003000000000003E+01	{~~}
332	START H	Gasifier	74	-0.2398848478333941E+04	{~~}
333	START M	Gasifier	3	-0.8527518947879474E-01	{~~}
334	START P		3	0.9980000000000002E+00	{~~}
335	START H	Gasifier	3	-0.3507877913073774E+04	{~~}
336	START M	Gasifier	99	-0.2653014000000009E-03	{~~}
337	START P		99	0.1013000000000003E+01	{~~}
338	START H	Gasifier	99	-0.4308000000000012E+04	{~~}
339	START Q	Gasifier	302	0.0000000000000000E+00	{~~}
340	START ZA	Gasifier	1	0.8500945239865266E+05	{~~}
341	START ZA	Gasifier	2	0.4363965291425185E+05	{~~}
342	START ZA	Gasifier	3	0.1172765217993689E+06	{~~}
343	START ZA	Gasifier	4	0.3124902840469581E+06	{~~}
344	START ZA	Gasifier	5	0.1827651987487794E+06	{~~}
345	START ZA	Gasifier	6	0.2292482774424778E+06	{~~}
346	START ZA	Gasifier	7	-0.3279719879436743E+06	{~~}
347	START Y_J	raw_PG	H2	0.2538114658675982E+00	{~~}
348	START Y_J	raw_PG	O2	0.0000000000000000E+00	{~~}
349	START Y_J	raw_PG	N2	0.2896541868376543E+00	{~~}
350	START Y_J	raw_PG	CO	0.1761818347160904E+00	{~~}
351	START Y_J	raw_PG	NO	0.0000000000000000E+00	{~~}
352	START Y_J	raw_PG	CO2	0.1144395150133747E+00	{~~}
353	START Y_J	raw_PG	H2O-G	0.1523098114753788E+00	{~~}
354	START Y_J	raw_PG	NH3	0.0000000000000000E+00	{~~}
355	START Y_J	raw_PG	H2S	0.4615796164902317E-04	{~~}
356	START Y_J	raw_PG	SO2	0.0000000000000000E+00	{~~}
357	START Y_J	raw_PG	CH4	0.1011293223314741E-01	{~~}
358	START Y_J	raw_PG	NO2	0.0000000000000000E+00	{~~}
359	START Y_J	raw_PG	HCN	0.0000000000000000E+00	{~~}
360	START Y_J	raw_PG	COS	0.0000000000000000E+00	{~~}
361	START Y_J	raw_PG	AR	0.3444095895110012E-02	{~~}
362	START X_J	Ash	C	0.0000000000000000E+00	{~~}
363	START X_J	Ash	ASH	0.1000000000000003E+01	{~~}
364	START M	airpreheat	3	0.8527518947879474E-01	{~~}
365	START H	airpreheat	3	-0.3507877913073774E+04	{~~}
366	START M	airpreheat	4	-0.8527518947879474E-01	{~~}
367	START P		4	0.9930000000000002E+00	{~~}
368	START H	airpreheat	4	-0.3918630307677507E+04	{~~}
369	START M	airpreheat	72	0.4254049087879462E-01	{~~}
370	START P		72	0.1008000000000003E+01	{~~}
371	START H	airpreheat	72	-0.9883454496688256E+02	{~~}
372	START M	airpreheat	73	-0.4254049087879462E-01	{~~}
373	START P		73	0.1003000000000003E+01	{~~}
374	START H	airpreheat	73	0.7245454291500146E+03	{~~}
375	START Q	airpreheat	303	0.0000000000000000E+00	{~~}
376	START ZA	airpreheat	1	0.3502698827870191E+02	{~~}
377	START M	steamheater	4	0.8527518947879474E-01	{~~}
378	START H	steamheater	4	-0.3918630307677508E+04	{~~}

```

379 START M steamheater 5 -0.8527518947879474E-01 {~~}
380 START P 5 0.9880000000000029E+00 {~~}
381 START H steamheater 5 -0.4375257198957320E+04 {~~}
382 START M steamheater 63 0.2000459030657081E+00 {~~}
383 START P 63 0.1003000000000003E+01 {~~}
384 START H steamheater 63 -0.1319118556200299E+05 {~~}
385 START M steamheater 64 -0.2000459030657081E+00 {~~}
386 START H steamheater 64 -0.1299653551379776E+05 {~~}
387 START Q steamheater 304 0.0000000000000000E+00 {~~}
388 START ZA steamheater 1 0.3893894467499886E+02 {~~}
389 START M steamblower 61 0.2123574820130765E+00 {~~}
390 START H steamblower 61 -0.1319443607829823E+05 {~~}
391 START M steamblower 62 -0.2123574820130765E+00 {~~}
392 START P 62 0.1003000000000003E+01 {~~}
393 START H steamblower 62 -0.1319118556200299E+05 {~~}
394 START Q steamblower 305 -0.1408717256529157E-01 {~~}
395 START W steamblower 105 0.7043586282645840E+00 {~~}
396 START M split1 62 0.2123574820130765E+00 {~~}
397 START H split1 62 -0.1319118556200299E+05 {~~}
398 START M split1 63 -0.2000459030657081E+00 {~~}
399 START H split1 63 -0.1319118556200299E+05 {~~}
400 START M split1 69 -0.1231157894736845E-01 {~~}
401 START P 69 0.1003000000000003E+01 {~~}
402 START H split1 69 -0.1319118556200299E+05 {~~}
403 START M mix1 73 0.4254049087879462E-01 {~~}
404 START H mix1 73 0.7245454291500146E+03 {~~}
405 START M mix1 69 0.1231157894736845E-01 {~~}
406 START H mix1 69 -0.1319118556200300E+05 {~~}
407 START M mix1 74 -0.5485206982616307E-01 {~~}
408 START H mix1 74 -0.2398848478333941E+04 {~~}
409 START Y_J humid_air H2 0.0000000000000000E+00 {~~}
410 START Y_J humid_air O2 0.1417803964772678E+00 {~~}
411 START Y_J humid_air N2 0.5281063539146039E+00 {~~}
412 START Y_J humid_air CO 0.0000000000000000E+00 {~~}
413 START Y_J humid_air NO 0.0000000000000000E+00 {~~}
414 START Y_J humid_air CO2 0.2049837057502668E-03 {~~}
415 START Y_J humid_air H2O-G 0.3236220989260391E+00 {~~}
416 START Y_J humid_air NH3 0.0000000000000000E+00 {~~}
417 START Y_J humid_air H2S 0.0000000000000000E+00 {~~}
418 START Y_J humid_air SO2 0.0000000000000000E+00 {~~}
419 START Y_J humid_air CH4 0.0000000000000000E+00 {~~}
420 START Y_J humid_air C2H6 0.0000000000000000E+00 {~~}
421 START Y_J humid_air C3H8 0.0000000000000000E+00 {~~}
422 START Y_J humid_air C4H10-N 0.0000000000000000E+00 {~~}
423 START Y_J humid_air C4H10-I 0.0000000000000000E+00 {~~}
424 START Y_J humid_air C5H12 0.0000000000000000E+00 {~~}
425 START Y_J humid_air C6H14 0.0000000000000000E+00 {~~}
426 START Y_J humid_air C7H16 0.0000000000000000E+00 {~~}
427 START Y_J humid_air C8H18 0.0000000000000000E+00 {~~}
428 START Y_J humid_air C2H4 0.0000000000000000E+00 {~~}
429 START Y_J humid_air C3H6 0.0000000000000000E+00 {~~}
430 START Y_J humid_air C5H10 0.0000000000000000E+00 {~~}
431 START Y_J humid_air C6H12-1 0.0000000000000000E+00 {~~}
432 START Y_J humid_air C7H14 0.0000000000000000E+00 {~~}
433 START Y_J humid_air C2H2 0.0000000000000000E+00 {~~}
434 START Y_J humid_air C6H6 0.0000000000000000E+00 {~~}
435 START Y_J humid_air C6H12-C 0.0000000000000000E+00 {~~}
436 START Y_J humid_air C 0.0000000000000000E+00 {~~}
437 START Y_J humid_air S 0.0000000000000000E+00 {~~}
438 START Y_J humid_air NO2 0.0000000000000000E+00 {~~}
439 START Y_J humid_air HCN 0.0000000000000000E+00 {~~}
440 START Y_J humid_air COS 0.0000000000000000E+00 {~~}
441 START Y_J humid_air N2O 0.0000000000000000E+00 {~~}
442 START Y_J humid_air NO3 0.0000000000000000E+00 {~~}
443 START Y_J humid_air SO3 0.0000000000000000E+00 {~~}
444 START Y_J humid_air AR 0.6286166976341515E-02 {~~}
445 START Y_J humid_air ASH 0.0000000000000000E+00 {~~}
446 START Y_J humid_air TAR 0.0000000000000000E+00 {~~}
447 START Y_J humid_air CH3OH 0.0000000000000000E+00 {~~}
448 START M gascooler 5 0.8527518947879474E-01 {~~}
449 START H gascooler 5 -0.4375257198957320E+04 {~~}
450 START M gascooler 6 -0.8527518947879474E-01 {~~}
451 START P 6 0.9830000000000029E+00 {~~}
452 START H gascooler 6 -0.4624611248324044E+04 {~~}
453 START M gascooler 98 0.0000000000000000E+00 {~~}
454 START P 98 0.9830000000000029E+00 {~~}

```

```

455 START H gascooler 98 -0.1559408877861429E+05 {~~}
456 START M gascooler 81 0.1016636501943121E+00 {~~}
457 START P 81 0.10130000000000003E+01 {~~}
458 START H gascooler 81 -0.1584524528596515E+05 {~~}
459 START M gascooler 82 -0.1016636501943121E+00 {~~}
460 START P 82 0.10080000000000003E+01 {~~}
461 START H gascooler 82 -0.1563608779686840E+05 {~~}
462 START Q gascooler 306 0.0000000000000000E+00 {~~}
463 START Y_J cold_PG H2 0.2538114658675977E+00 {~~}
464 START Y_J cold_PG O2 0.0000000000000000E+00 {~~}
465 START Y_J cold_PG N2 0.2896541868376540E+00 {~~}
466 START Y_J cold_PG CO 0.1761818347160901E+00 {~~}
467 START Y_J cold_PG NO 0.0000000000000000E+00 {~~}
468 START Y_J cold_PG CO2 0.1144395150133745E+00 {~~}
469 START Y_J cold_PG H2O-G 0.1523098114753788E+00 {~~}
470 START Y_J cold_PG NH3 0.0000000000000000E+00 {~~}
471 START Y_J cold_PG H2S 0.4615796164902310E-04 {~~}
472 START Y_J cold_PG SO2 0.0000000000000000E+00 {~~}
473 START Y_J cold_PG CH4 0.1011293223314739E-01 {~~}
474 START Y_J cold_PG C2H6 0.0000000000000000E+00 {~~}
475 START Y_J cold_PG C3H8 0.0000000000000000E+00 {~~}
476 START Y_J cold_PG C4H10-N 0.0000000000000000E+00 {~~}
477 START Y_J cold_PG C4H10-I 0.0000000000000000E+00 {~~}
478 START Y_J cold_PG C5H12 0.0000000000000000E+00 {~~}
479 START Y_J cold_PG C6H14 0.0000000000000000E+00 {~~}
480 START Y_J cold_PG C7H16 0.0000000000000000E+00 {~~}
481 START Y_J cold_PG C8H18 0.0000000000000000E+00 {~~}
482 START Y_J cold_PG C2H4 0.0000000000000000E+00 {~~}
483 START Y_J cold_PG C3H6 0.0000000000000000E+00 {~~}
484 START Y_J cold_PG C5H10 0.0000000000000000E+00 {~~}
485 START Y_J cold_PG C6H12-1 0.0000000000000000E+00 {~~}
486 START Y_J cold_PG C7H14 0.0000000000000000E+00 {~~}
487 START Y_J cold_PG C2H2 0.0000000000000000E+00 {~~}
488 START Y_J cold_PG C6H6 0.0000000000000000E+00 {~~}
489 START Y_J cold_PG C6H12-C 0.0000000000000000E+00 {~~}
490 START Y_J cold_PG C 0.0000000000000000E+00 {~~}
491 START Y_J cold_PG S 0.0000000000000000E+00 {~~}
492 START Y_J cold_PG NO2 0.0000000000000000E+00 {~~}
493 START Y_J cold_PG HCN 0.0000000000000000E+00 {~~}
494 START Y_J cold_PG COS 0.0000000000000000E+00 {~~}
495 START Y_J cold_PG N2O 0.0000000000000000E+00 {~~}
496 START Y_J cold_PG NO3 0.0000000000000000E+00 {~~}
497 START Y_J cold_PG SO3 0.0000000000000000E+00 {~~}
498 START Y_J cold_PG AR 0.3444095895110008E-02 {~~}
499 START M gasclean 6 0.8527518947879474E-01 {~~}
500 START H gasclean 6 -0.4624611248324044E+04 {~~}
501 START M gasclean 7 -0.8526899202586896E-01 {~~}
502 START P 7 0.97810000000000029E+00 {~~}
503 START H gasclean 7 -0.4624908439609428E+04 {~~}
504 START M gasclean 97 -0.6197452925764212E-05 {~~}
505 START P 97 0.97810000000000029E+00 {~~}
506 START H gasclean 97 -0.5356408846834941E+03 {~~}
507 START Q gasclean 307 0.0000000000000000E+00 {~~}
508 START Y_J clean_PG H2 0.2538231818282905E+00 {~~}
509 START Y_J clean_PG O2 0.0000000000000000E+00 {~~}
510 START Y_J clean_PG N2 0.2896675573016552E+00 {~~}
511 START Y_J clean_PG CO 0.1761899672858432E+00 {~~}
512 START Y_J clean_PG NO 0.0000000000000000E+00 {~~}
513 START Y_J clean_PG CO2 0.1144447975519510E+00 {~~}
514 START Y_J clean_PG H2O-G 0.1523168421103356E+00 {~~}
515 START Y_J clean_PG CH4 0.1011339904703276E-01 {~~}
516 START Y_J clean_PG NO2 0.0000000000000000E+00 {~~}
517 START Y_J clean_PG AR 0.3444254874894436E-02 {~~}
518 START Y_J impurities H2O-G 0.0000000000000000E+00 {~~}
519 START Y_J impurities NH3 0.0000000000000000E+00 {~~}
520 START Y_J impurities H2S 0.10000000000000003E+01 {~~}
521 START Y_J impurities SO2 0.0000000000000000E+00 {~~}
522 START Y_J impurities HCN 0.0000000000000000E+00 {~~}
523 START Y_J impurities COS 0.0000000000000000E+00 {~~}
524 START Y_J impurities AR 0.0000000000000000E+00 {~~}
525 START Y_J impurities ASH 0.0000000000000000E+00 {~~}
526 START M condenser 7 0.8526899202586896E-01 {~~}
527 START H condenser 7 -0.4624908439609428E+04 {~~}
528 START M condenser 8 -0.8320484335731909E-01 {~~}
529 START P 8 0.97310000000000029E+00 {~~}
530 START H condenser 8 -0.4466561290262767E+04 {~~}

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DNA Input for SOFC-MGT scenario

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531	START M	condenser	96	-0.2064148668549882E-02	{~~}
532	START P		96	0.9731000000000029E+00	{~~}
533	START H	condenser	96	-0.1576166949955457E+05	{~~}
534	START M	condenser	83	0.4691527326491425E-01	{~~}
535	START P		83	0.1013000000000003E+01	{~~}
536	START H	condenser	83	-0.1584524528596515E+05	{~~}
537	START M	condenser	84	-0.4691527326491425E-01	{~~}
538	START P		84	0.1008000000000003E+01	{~~}
539	START H	condenser	84	-0.1563608779686840E+05	{~~}
540	START Q	condenser	308	0.0000000000000000E+00	{~~}
541	START Y_J	dry_PG	H2	0.2614256920940570E+00	{~~}
542	START Y_J	dry_PG	O2	0.0000000000000000E+00	{~~}
543	START Y_J	dry_PG	N2	0.2983436780648686E+00	{~~}
544	START Y_J	dry_PG	CO	0.1814672080223565E+00	{~~}
545	START Y_J	dry_PG	NO	0.0000000000000000E+00	{~~}
546	START Y_J	dry_PG	CO2	0.1178726473723857E+00	{~~}
547	START Y_J	dry_PG	H2O-G	0.1269270417636784E+00	{~~}
548	START Y_J	dry_PG	NH3	0.0000000000000000E+00	{~~}
549	START Y_J	dry_PG	H2S	0.0000000000000000E+00	{~~}
550	START Y_J	dry_PG	SO2	0.0000000000000000E+00	{~~}
551	START Y_J	dry_PG	CH4	0.1041631550849636E-01	{~~}
552	START Y_J	dry_PG	C2H6	0.0000000000000000E+00	{~~}
553	START Y_J	dry_PG	C3H8	0.0000000000000000E+00	{~~}
554	START Y_J	dry_PG	C4H10-N	0.0000000000000000E+00	{~~}
555	START Y_J	dry_PG	C4H10-I	0.0000000000000000E+00	{~~}
556	START Y_J	dry_PG	C5H12	0.0000000000000000E+00	{~~}
557	START Y_J	dry_PG	C6H14	0.0000000000000000E+00	{~~}
558	START Y_J	dry_PG	C7H16	0.0000000000000000E+00	{~~}
559	START Y_J	dry_PG	C8H18	0.0000000000000000E+00	{~~}
560	START Y_J	dry_PG	C2H4	0.0000000000000000E+00	{~~}
561	START Y_J	dry_PG	C3H6	0.0000000000000000E+00	{~~}
562	START Y_J	dry_PG	C5H10	0.0000000000000000E+00	{~~}
563	START Y_J	dry_PG	C6H12-1	0.0000000000000000E+00	{~~}
564	START Y_J	dry_PG	C7H14	0.0000000000000000E+00	{~~}
565	START Y_J	dry_PG	C2H2	0.0000000000000000E+00	{~~}
566	START Y_J	dry_PG	C6H6	0.0000000000000000E+00	{~~}
567	START Y_J	dry_PG	C6H12-C	0.0000000000000000E+00	{~~}
568	START Y_J	dry_PG	C	0.0000000000000000E+00	{~~}
569	START Y_J	dry_PG	S	0.0000000000000000E+00	{~~}
570	START Y_J	dry_PG	NO2	0.0000000000000000E+00	{~~}
571	START Y_J	dry_PG	HCN	0.0000000000000000E+00	{~~}
572	START Y_J	dry_PG	COS	0.0000000000000000E+00	{~~}
573	START Y_J	dry_PG	N2O	0.0000000000000000E+00	{~~}
574	START Y_J	dry_PG	NO3	0.0000000000000000E+00	{~~}
575	START Y_J	dry_PG	SO3	0.0000000000000000E+00	{~~}
576	START Y_J	dry_PG	AR	0.3547417174159975E-02	{~~}
577	START M	PGcompressor	8	0.8320484335731909E-01	{~~}
578	START H	PGcompressor	8	-0.4466561290262767E+04	{~~}
579	START M	PGcompressor	9	-0.8320484335731909E-01	{~~}
580	START P		9	0.2505000000000006E+01	{~~}
581	START H	PGcompressor	9	-0.4289316158106304E+04	{~~}
582	START Q	PGcompressor	309	-0.3009725195290968E+00	{~~}
583	START W	PGcompressor	117	0.1504862597645489E+02	{~~}
584	START M	PGpreheat	11	0.1084136464468042E+00	{~~}
585	START P		11	0.2495000000000006E+01	{~~}
586	START H	PGpreheat	11	-0.6150750931339399E+04	{~~}
587	START M	PGpreheat	12	-0.1084136464468042E+00	{~~}
588	START P		12	0.2490000000000006E+01	{~~}
589	START H	PGpreheat	12	-0.6717227933915665E+04	{~~}
590	START M	PGpreheat	9	0.8320484335731909E-01	{~~}
591	START H	PGpreheat	9	-0.4289316158106304E+04	{~~}
592	START M	PGpreheat	10	-0.8320484335731909E-01	{~~}
593	START P		10	0.2500000000000006E+01	{~~}
594	START H	PGpreheat	10	-0.3551212040611485E+04	{~~}
595	START Q	PGpreheat	311	0.0000000000000000E+00	{~~}
596	START ZA	PGpreheat	1	0.6141383747754848E+02	{~~}
597	START M	aircompressor	31	0.7206544633491334E+00	{~~}
598	START P		31	0.1013000000000003E+01	{~~}
599	START H	aircompressor	31	-0.9883454496688256E+02	{~~}
600	START M	aircompressor	32	-0.7206544633491334E+00	{~~}
601	START P		32	0.2530000000000007E+01	{~~}
602	START H	aircompressor	32	0.1694338091721306E+02	{~~}
603	START Q	aircompressor	312	-0.1702773041748533E+01	{~~}
604	START W	aircompressor	117	0.8513865208742698E+02	{~~}
605	START M	airpreheat2	35	0.6954456602596484E+00	{~~}
606	START P		35	0.2500000000000006E+01	{~~}

DNA Input for SOFC-MGT scenario

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607 START H    airpreheat2      35  0.7462281704415040E+03 {~~}
608 START M    airpreheat2      36 -0.6954456602596484E+00 {~~}
609 START P    36  0.2490000000000000E+01 {~~}
610 START H    airpreheat2      36  0.6125054264003596E+03 {~~}
611 START M    airpreheat2      33  0.7206544633491334E+00 {~~}
612 START P    33  0.2520000000000007E+01 {~~}
613 START H    airpreheat2      33  0.3903614949152461E+03 {~~}
614 START M    airpreheat2      34 -0.7206544633491334E+00 {~~}
615 START P    34  0.2510000000000007E+01 {~~}
616 START H    airpreheat2      34  0.5194065598541856E+03 {~~}
617 START Q    airpreheat2     314  0.0000000000000000E+00 {~~}
618 START ZA   airpreheat2      1  0.9299690202142516E+02 {~~}
619 START M    sofc            10  0.8320484335731909E-01 {~~}
620 START H    sofc            10 -0.3551212040611485E+04 {~~}
621 START M    sofc            34  0.7206544633491334E+00 {~~}
622 START H    sofc            34  0.5194065598541854E+03 {~~}
623 START M    sofc            11 -0.1084136464468042E+00 {~~}
624 START H    sofc            11 -0.6150750931339399E+04 {~~}
625 START M    sofc            35 -0.6954456602596484E+00 {~~}
626 START H    sofc            35  0.7462281704415040E+03 {~~}
627 START E    sofc           215 -0.2266988082395728E+03 {~~}
628 START Q    sofc          315  0.0000000000000000E+00 {~~}
629 START ZA   sofc            1  0.8953504439170833E+05 {~~}
630 START ZA   sofc            2  0.7759617742337787E+05 {~~}
631 START ZA   sofc            3  0.1131334605653419E+06 {~~}
632 START ZA   sofc            4  0.2874557392272268E+06 {~~}
633 START ZA   sofc            5 -0.4346595838206942E+06 {~~}
634 START ZA   sofc            6  0.7031243231141652E+00 {~~}
635 START ZA   sofc            7  0.8490526863609010E+00 {~~}
636 START ZA   sofc            8  0.8500000000000002E+00 {~~}
637 START ZA   sofc            9  0.5074411560779050E+00 {~~}
638 START ZA   sofc           10  0.4097643685146410E+00 {~~}
639 START ZA   sofc           11  0.9653081902361105E+00 {~~}
640 START ZA   sofc           12  0.1081368457960910E+00 {~~}
641 START ZA   sofc           13  0.7147434745365800E-02 {~~}
642 START ZA   sofc           14  0.3042639760850667E-01 {~~}
643 START ZA   sofc           15  0.8195975120861470E+00 {~~}
644 START ZA   sofc           16 -0.8643528923812226E+05 {~~}
645 START ZA   sofc           17 -0.1885369880714487E+06 {~~}
646 START ZA   sofc           18 -0.1862755214698623E+06 {~~}
647 START ZA   sofc           19  0.6834375642423529E+00 {~~}
648 START ZA   sofc           20  0.2335762988681633E-01 {~~}
649 START ZA   sofc           21  0.1013478073726875E+04 {~~}
650 START ZA   sofc           22  0.3000000000000009E+03 {~~}
651 START ZA   sofc           23  0.9500000000000024E+00 {~~}
652 START Y_J  USED FUEL      H2    0.3681263343705554E-01 {~~}
653 START Y_J  USED FUEL      CO    0.2592602480079992E-01 {~~}
654 START Y_J  USED FUEL      CO2   0.2785668687819785E+00 {~~}
655 START Y_J  USED FUEL      H2O-G 0.3654198955141020E+00 {~~}
656 START Y_J  USED FUEL      CH4   0.1320885926659904E-06 {~~}
657 START Y_J  USED FUEL      N2    0.2932744453774739E+00 {~~}
658 START Y_J  USED FUEL      O2    0.1816887511884419E+00 {~~}
659 START Y_J  USED AIR       N2    0.7980728885885872E+00 {~~}
660 START Y_J  USED AIR       CO2   0.3097708197393921E-03 {~~}
661 START Y_J  USED AIR       H2O-G 0.1042895093122620E-01 {~~}
662 START Y_J  USED AIR       AR    0.9499638472008036E-02 {~~}
663 START M    burner          36  0.6954456602596484E+00 {~~}
664 START H    burner          36  0.6125054264003596E+03 {~~}
665 START M    burner          12  0.1084136464468042E+00 {~~}
666 START H    burner          12 -0.6717227933915663E+04 {~~}
667 START M    burner          41 -0.8038593067064525E+00 {~~}
668 START P    41  0.2488441260000007E+01 {~~}
669 START H    burner          41 -0.3760296498811286E+03 {~~}
670 START Q    burner          316  0.0000000000000000E+00 {~~}
671 START ZA   burner          1  0.3599992793955970E+02 {~~}
672 START Y_J  FLUE_GAS       O2    0.1528256566367803E+00 {~~}
673 START Y_J  FLUE_GAS       N2    0.7312927409586391E+00 {~~}
674 START Y_J  FLUE_GAS       NO    0.0000000000000000E+00 {~~}
675 START Y_J  FLUE_GAS       CO2   0.4265157978005395E-01 {~~}
676 START Y_J  FLUE_GAS       H2O-G 0.6501119656074644E-01 {~~}
677 START Y_J  FLUE_GAS       SO2   0.0000000000000000E+00 {~~}
678 START Y_J  FLUE_GAS       NO2   0.0000000000000000E+00 {~~}
679 START Y_J  FLUE_GAS       AR    0.8218826063782632E-02 {~~}
680 START M    GT              41  0.8038593067064525E+00 {~~}
681 START H    GT              41 -0.3760296498811286E+03 {~~}
682 START M    GT              42 -0.8038593067064525E+00 {~~}

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DNA Input for SOFC-MGT scenario

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683 START P          42  0.1033000000000003E+01 {~~}
684 START H          42  -0.5641539005908002E+03 {~~}
685 START W          117 -0.1512254297501471E+03 {~~}
686 START E          217 -0.4848624410195209E+02 {~~}
687 START Q          317 -0.2551907584313264E+01 {~~}
688 START W          117  0.5103815168626537E+02 {~~}
689 START M          42  0.8038593067064525E+00 {~~}
690 START H          42  -0.5641539005908002E+03 {~~}
691 START M          43  -0.8038593067064525E+00 {~~}
692 START P          43  0.1023000000000003E+01 {~~}
693 START H          43  -0.8989207289437225E+03 {~~}
694 START M          32  0.7206544633491334E+00 {~~}
695 START H          32  0.1694338091721306E+02 {~~}
696 START M          33  -0.7206544633491334E+00 {~~}
697 START H          33  0.3903614949152461E+03 {~~}
698 START Q          318 0.0000000000000000E+00 {~~}
699 START ZA          1  0.2691054305480973E+03 {~~}
700 START M          43  0.8038593067064525E+00 {~~}
701 START H          43  -0.8989207289437225E+03 {~~}
702 START M          44  -0.8038593067064525E+00 {~~}
703 START P          44  0.1013000000000003E+01 {~~}
704 START H          44  -0.1031734334544724E+04 {~~}
705 START M          85  0.5104452792040437E+00 {~~}
706 START P          85  0.1013000000000003E+01 {~~}
707 START H          85  -0.1584524528596515E+05 {~~}
708 START M          86  -0.5104452792040437E+00 {~~}
709 START P          86  0.1008000000000003E+01 {~~}
710 START H          86  -0.1563608779686840E+05 {~~}
711 START Q          319 0.0000000000000000E+00 {~~}
712 START ZA          1  0.1067634529196043E+03 {~~}
713 C ~~~~~
714 C ~~ End of generated initial guesses.
715 C ~~~~~
end

```

DNA Output for SOFC–MGT scenario

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1	Biomass gasification (Viking) + SOFC/MGT incl. recuperation												
2	RUN NUMBER 1												
3													
4													
5													
6	ALGEBRAIC VARIABLES												
7	NO	TO	MEDIA	M	T	P	H	ENERGY	X	S	V	U	
8	DE	COMPONENT		[kg/s]	[C]	[bar]	[kJ/kg]	[kJ/s]		[kJ/kg K]	[m3/kg]	[kJ/kg]	
9	-----												
10	1	Dryer	Wood	0.04	15.00	-	-8621.6	4.991E+02	-	0.4612	-	-8621.6	
11	64	Dryer	STEAM-HF	0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2	
12	2	Dryer	DryWood	-0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1	
13	61	Dryer	STEAM-HF	-0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1	
14	301	Dryer	HEAT					0.000E+00					
15	2	Gasifier	DryWood	0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1	
16	26	Gasifier	STEAM-HF	0.00	150.00	1.003	-13194.5		-	11.1292	1.9309	-13388.2	
17	74	Gasifier	humid_air	0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7	
18	3	Gasifier	raw_PG	-0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1	
19	99	Gasifier	Ash	0.00	800.00	-	-4308.0		-	0.0000	-	-4308.0	
20	302	Gasifier	HEAT					0.000E+00					
21	3	airpreheat	raw_PG	0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1	
22	4	airpreheat	raw_PG	-0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7	
23	72	airpreheat	STANDARD_AIR	0.04	15.00	1.008	-98.8		-	6.8668	0.8237	-181.9	
24	73	airpreheat	STANDARD_AIR	-0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1	
25	303	airpreheat	HEAT					0.000E+00					
26	4	steamheater	raw_PG	0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7	
27	5	steamheater	raw_PG	-0.09	259.48	0.988	-4375.3		-	9.7468	2.0710	-4579.9	
28	63	steamheater	STEAM-HF	0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
29	64	steamheater	STEAM-HF	-0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2	
30	304	steamheater	HEAT					0.000E+00					
31	61	steamblower	STEAM-HF	0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1	
32	62	steamblower	STEAM-HF	-0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
33	305	steamblower	HEAT					-1.409E-02					
34	105	steamblower	MECH_POWER					7.044E-01					
35	62	split1	STEAM-HF	0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
36	63	split1	STEAM-HF	-0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
37	69	split1	STEAM-HF	-0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
38	73	mix1	STANDARD_AIR	0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1	
39	69	mix1	STEAM-HF	0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
40	74	mix1	humid_air	-0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7	
41	5	gascooler	raw_PG	0.09	259.48	0.988	-4375.3		-	9.7468	2.0710	-4579.9	
42	6	gascooler	cold_PG	-0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1	
43	98	gascooler	STEAM-HF	0.00	90.00	0.983	-15594.1		-	4.7085	0.0010	-15594.2	
44	81	gascooler	STEAM-HF	0.10	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3	
45	82	gascooler	STEAM-HF	-0.10	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2	
46	306	gascooler	HEAT					0.000E+00					
47	6	gasclean	cold_PG	0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1	
48	7	gasclean	clean_PG	-0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4	
49	97	gasclean	impurities	0.00	90.00	0.978	-535.6		-	6.2438	0.9059	-624.2	
50	307	gasclean	HEAT					0.000E+00					
51	7	condenser	clean_PG	0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4	
52	8	condenser	dry_PG	-0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1	
53	96	condenser	STEAM-HF	0.00	50.01	0.973	-15761.7		-	4.2198	0.0010	-15761.7	
54	83	condenser	STEAM-HF	0.05	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3	

DNA Output for SOFC-MGT scenario

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54												
55	84	condenser	STEAM-HF	-0.05	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
56	308	condenser	HEAT					0.000E+00				
57	8	PGcompressor	dry_PG	0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1
58	9	PGcompressor	dry_PG	-0.08	173.32	2.505	-4289.3		-	9.0626	0.6813	-4460.0
59	309	PGcompressor	HEAT					-3.010E-01				
60	117	PGcompressor	MECH_POWER					1.505E+01				
61	11	PGpreheat	USED_FUEL	0.11	800.00	2.495	-6150.8		-	8.8073	1.2836	-6471.0
62	12	PGpreheat	USED_FUEL	-0.11	409.82	2.490	-6717.2		-	8.1544	0.8186	-6921.1
63	9	PGpreheat	dry_PG	0.08	173.32	2.505	-4289.3		-	9.0626	0.6813	-4460.0
64	10	PGpreheat	dry_PG	-0.08	650.00	2.500	-3551.2		-	10.1804	1.4115	-3904.1
65	311	PGpreheat	HEAT					0.000E+00				
66	31	aircompressor	STANDARD_AIR	0.72	15.00	1.013	-98.8		-	6.8653	0.8196	-181.9
67	32	aircompressor	STANDARD_AIR	-0.72	129.26	2.530	16.9		-	6.9399	0.4583	-99.0
68	312	aircompressor	HEAT					-1.703E+00				
69	117	aircompressor	MECH_POWER					8.514E+01				
70	42	recuperator	FLUE_GAS	0.80	546.00	1.033	-564.2		-	8.0822	2.2930	-801.0
71	43	recuperator	FLUE_GAS	-0.80	245.28	1.023	-898.9		-	7.5771	1.4654	-1048.8
72	32	recuperator	STANDARD_AIR	0.72	129.26	2.530	16.9		-	6.9399	0.4583	-99.0
73	33	recuperator	STANDARD_AIR	-0.72	483.49	2.520	390.4		-	7.6042	0.8652	172.3
74	318	recuperator	HEAT					0.000E+00				
75	35	airpreheat2	USED_AIR	0.70	800.00	2.500	746.2		-	8.0049	1.2413	435.9
76	36	airpreheat2	USED_AIR	-0.70	683.95	2.490	612.5		-	7.8742	1.1115	335.7
77	33	airpreheat2	STANDARD_AIR	0.72	483.49	2.520	390.4		-	7.6042	0.8652	172.3
78	34	airpreheat2	STANDARD_AIR	-0.72	600.00	2.510	519.4		-	7.7639	1.0024	267.8
79	314	airpreheat2	HEAT					0.000E+00				
80	10	sofc	dry_PG	0.08	650.00	2.500	-3551.2		-	10.1804	1.4115	-3904.1
81	34	sofc	STANDARD_AIR	0.72	600.00	2.510	519.4		-	7.7639	1.0024	267.8
82	11	sofc	USED_FUEL	-0.11	800.00	2.495	-6150.8		-	8.8073	1.2836	-6471.0
83	35	sofc	USED_AIR	-0.70	800.00	2.500	746.2		-	8.0049	1.2413	435.9
84	215	sofc	ELECT_POWER					-2.267E+02				
85	315	sofc	HEAT					0.000E+00				
86	36	burner	USED_AIR	0.70	683.95	2.490	612.5		-	7.8742	1.1115	335.7
87	12	burner	USED_FUEL	0.11	409.82	2.490	-6717.2		-	8.1544	0.8186	-6921.1
88	41	burner	FLUE_GAS	-0.80	706.46	2.488	-376.0		-	8.0376	1.1383	-659.3
89	316	burner	HEAT					0.000E+00				
90	41	GT	FLUE_GAS	0.80	706.46	2.488	-376.0		-	8.0376	1.1383	-659.3
91	42	GT	FLUE_GAS	-0.80	546.00	1.033	-564.2		-	8.0822	2.2930	-801.0
92	117	GT	MECH_POWER					-1.512E+02				
93	217	generator	ELECT_POWER					-4.849E+01				
94	317	generator	HEAT					-2.552E+00				
95	117	generator	MECH_POWER					5.104E+01				
96	43	exhaustcooler	FLUE_GAS	0.80	245.28	1.023	-898.9		-	7.5771	1.4654	-1048.8
97	44	exhaustcooler	FLUE_GAS	-0.80	120.02	1.013	-1031.7		-	7.2869	1.1223	-1145.4
98	85	exhaustcooler	STEAM-HF	0.51	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3
99	86	exhaustcooler	STEAM-HF	-0.51	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
100	319	exhaustcooler	HEAT					0.000E+00				

101

102

103

104 EXERGY

105

106 NO | TO | MEDIA | E_PH | E_CH | E | EX_PH | EX_CH | EX |

107 DE | COMPONENT | [kJ/kg] | [kJ/kg] | [kJ/kg] | [kJ/s] | [kJ/s] | [kJ/s] |

DNA Output for SOFC–MGT scenario

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109	1	Dryer	Wood		0.00		13311.33		13311.33		0.00		572.39		572.39	
110	64	Dryer	STEAM-HF		660.71		-		660.71		132.17		-		132.17	
111	2	Dryer	DryWood		-54.56		18651.57		18597.01		1.67		-572.39		-570.71	
112	61	Dryer	STEAM-HF		583.11		-		583.11		-123.83		-		-123.83	
113	301	Dryer	HEAT		-		-		-		0.00		0.00		0.00	
114	2	Gasifier	DryWood		-54.56		18651.57		18597.01		-1.67		572.39		570.71	
115	26	Gasifier	STEAM-HF		584.41		-		584.41		0.00		-		0.00	
116	74	Gasifier	humid_air		310.33		66.40		376.73		17.02		3.64		20.66	
117	3	Gasifier	raw_PG		644.70		5438.32		6083.02		-54.98		-463.75		-518.73	
118	99	Gasifier	Ash		785.00		-		785.00		-0.21		-		-0.21	
119	302	Gasifier	HEAT		-		-		-		0.00		0.00		0.00	
120	3	airpreheat	raw_PG		644.70		5438.32		6083.02		54.98		463.75		518.73	
121	4	airpreheat	raw_PG		358.65		5438.32		5796.96		-30.58		-463.75		-494.34	
122	72	airpreheat	STANDARD_AIR		0.66		3.73		4.39		0.03		0.16		0.19	
123	73	airpreheat	STANDARD_AIR		427.84		3.73		431.57		-18.20		-0.16		-18.36	
124	303	airpreheat	HEAT		-		-		-		0.00		0.00		0.00	
125	4	steamheater	raw_PG		358.65		5438.32		5796.96		30.58		463.75		494.34	
126	5	steamheater	raw_PG		97.80		5438.32		5536.12		-8.34		-463.75		-472.09	
127	63	steamheater	STEAM-HF		585.47		-		585.47		117.12		-		117.12	
128	64	steamheater	STEAM-HF		660.71		-		660.71		-132.17		-		-132.17	
129	304	steamheater	HEAT		-		-		-		0.00		0.00		0.00	
130	61	steamblower	STEAM-HF		583.11		-		583.11		123.83		-		123.83	
131	62	steamblower	STEAM-HF		585.47		-		585.47		-124.33		-		-124.33	
132	305	steamblower	HEAT		-		-		-		0.00		0.00		0.00	
133	105	steamblower	MECH_POWER		-		-		-		0.70		0.00		0.70	
134	62	split1	STEAM-HF		585.47		-		585.47		124.33		-		124.33	
135	63	split1	STEAM-HF		585.47		-		585.47		-117.12		-		-117.12	
136	69	split1	STEAM-HF		585.47		-		585.47		-7.21		-		-7.21	
137	73	mix1	STANDARD_AIR		427.84		3.73		431.57		18.20		0.16		18.36	
138	69	mix1	STEAM-HF		585.47		-		585.47		7.21		-		7.21	
139	74	mix1	humid_air		310.33		66.40		376.73		-17.02		-3.64		-20.66	
140	5	gascooler	raw_PG		97.80		5438.32		5536.12		8.34		463.75		472.09	
141	6	gascooler	cold_PG		10.04		5438.32		5448.36		-0.86		-463.75		-464.61	
142	98	gascooler	STEAM-HF		34.93		-		34.93		0.00		-		0.00	
143	81	gascooler	STEAM-HF		1.49		-		1.49		0.15		-		0.15	
144	82	gascooler	STEAM-HF		26.73		-		26.73		-2.72		-		-2.72	
145	306	gascooler	HEAT		-		-		-		0.00		0.00		0.00	
146	6	gasclean	cold_PG		10.04		5438.32		5448.36		0.86		463.75		464.61	
147	7	gasclean	clean_PG		9.49		5437.03		5446.52		-0.81		-463.61		-464.42	
148	97	gasclean	impurities		6.93		23829.09		23836.02		0.00		-0.15		-0.15	
149	307	gasclean	HEAT		-		-		-		0.00		0.00		0.00	
150	7	condenser	clean_PG		9.49		5437.03		5446.52		0.81		463.61		464.42	
151	8	condenser	dry_PG		-0.23		5566.16		5565.93		0.02		-463.13		-463.11	
152	96	condenser	STEAM-HF		8.19		-		8.19		-0.02		-		-0.02	
153	83	condenser	STEAM-HF		1.49		-		1.49		0.07		-		0.07	
154	84	condenser	STEAM-HF		26.73		-		26.73		-1.25		-		-1.25	
155	308	condenser	HEAT		-		-		-		0.00		0.00		0.00	
156	8	PGcompressor	dry_PG		-0.23		5566.16		5565.93		-0.02		463.13		463.11	
157	9	PGcompressor	dry_PG		147.40		5566.16		5713.56		-12.26		-463.13		-475.40	
158	309	PGcompressor	HEAT		-		-		-		0.00		0.00		0.00	
159	117	PGcompressor	MECH_POWER		-		-		-		15.05		0.00		15.05	
160	11	PGpreheat	USED_FUEL		646.94		787.09		1434.03		70.14		85.33		155.47	
161	12	PGpreheat	USED_FUEL		268.59		787.09		1055.68		-29.12		-85.33		-114.45	

DNA Output for SOFC-MGT scenario

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162	9	PGpreheat	dry_PG		147.40		5566.16		5713.56		12.26		463.13		475.40
163	10	PGpreheat	dry_PG		563.40		5566.16		6129.56		-46.88		-463.13		-510.01
164	311	PGpreheat	HEAT		-		-		-		0.00		0.00		0.00
165	31	aircompressor	STANDARD_AIR		1.07		3.73		4.81		0.77		2.69		3.46
166	32	aircompressor	STANDARD_AIR		95.36		3.73		99.09		-68.72		-2.69		-71.41
167	312	aircompressor	HEAT		-		-		-		0.00		0.00		0.00
168	117	aircompressor	MECH_POWER		-		-		-		85.14		0.00		85.14
169	42	recuperator	FLUE_GAS		255.61		21.61		277.21		205.47		17.37		222.84
170	43	recuperator	FLUE_GAS		66.38		21.61		87.98		-53.36		-17.37		-70.73
171	32	recuperator	STANDARD_AIR		95.36		3.73		99.09		68.72		2.69		71.41
172	33	recuperator	STANDARD_AIR		277.36		3.73		281.10		-199.88		-2.69		-202.57
173	318	recuperator	HEAT		-		-		-		0.00		0.00		0.00
174	35	airpreheat2	USEDAIR		521.69		3.79		525.48		362.81		2.63		365.44
175	36	airpreheat2	USEDAIR		425.63		3.79		429.42		-296.00		-2.63		-298.64
176	33	airpreheat2	STANDARD_AIR		277.36		3.73		281.10		199.88		2.69		202.57
177	34	airpreheat2	STANDARD_AIR		360.38		3.73		364.12		-259.71		-2.69		-262.40
178	314	airpreheat2	HEAT		-		-		-		0.00		0.00		0.00
179	10	sofc	dry_PG		563.40		5566.16		6129.56		46.88		463.13		510.01
180	34	sofc	STANDARD_AIR		360.38		3.73		364.12		259.71		2.69		262.40
181	11	sofc	USEDFUEL		646.94		787.09		1434.03		-70.14		-85.33		-155.47
182	35	sofc	USEDAIR		521.69		3.79		525.48		-362.81		-2.63		-365.44
183	215	sofc	ELECT_POWER		-		-		-		-226.70		0.00		-226.70
184	315	sofc	HEAT		-		-		-		0.00		0.00		0.00
185	36	burner	USEDAIR		425.63		3.79		429.42		296.00		2.63		298.64
186	12	burner	USEDFUEL		268.59		787.09		1055.68		29.12		85.33		114.45
187	41	burner	FLUE_GAS		456.58		21.61		478.19		-367.03		-17.37		-384.40
188	316	burner	HEAT		-		-		-		0.00		0.00		0.00
189	41	GT	FLUE_GAS		456.58		21.61		478.19		367.03		17.37		384.40
190	42	GT	FLUE_GAS		255.61		21.61		277.21		-205.47		-17.37		-222.84
191	117	GT	MECH_POWER		-		-		-		-151.23		0.00		-151.23
192	217	generator	ELECT_POWER		-		-		-		-48.49		0.00		-48.49
193	317	generator	HEAT		-		-		-		0.00		0.00		0.00
194	117	generator	MECH_POWER		-		-		-		51.04		0.00		51.04
195	43	exhaustcooler	FLUE_GAS		66.38		21.61		87.98		53.36		17.37		70.73

DNA Output for SOFC–MGT scenario

5/7

215 IDEAL GAS COMPOSITION (MOLAR BASE):

216

	humid_air	raw_PG	STANDARD_AIR	cold_PG	clean_PG	
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218 -----

219	HYDROGEN	0.0000E+00	0.2538E+00	0.0000E+00	0.2538E+00	0.2538E+00	
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220	OXYGEN	0.1418E+00	0.0000E+00	0.2075E+00	0.0000E+00	0.0000E+00	
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221	NITROGEN	0.5281E+00	0.2897E+00	0.7729E+00	0.2897E+00	0.2897E+00	
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222	CARBON MONOXIDE	0.0000E+00	0.1762E+00	0.0000E+00	0.1762E+00	0.1762E+00	
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223	CARBON DIOXIDE	0.2050E-03	0.1144E+00	0.3000E-03	0.1144E+00	0.1144E+00	
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224	WATER (I.G.)	0.3236E+00	0.1523E+00	0.1010E-01	0.1523E+00	0.1523E+00	
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225	HYDROGEN SULFIDE	0.0000E+00	0.4616E-04	0.0000E+00	0.4616E-04	0.0000E+00	
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226	METHANE	0.0000E+00	0.1011E-01	0.0000E+00	0.1011E-01	0.1011E-01	
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227	ARGON	0.6286E-02	0.3444E-02	0.9200E-02	0.3444E-02	0.3444E-02	
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228 -----

229	MEAN MOLE MASS	0.2542E+02	0.2164E+02	0.2885E+02	0.2164E+02	0.2164E+02	
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230	NET CALORI VALUE	0.0000E+00	0.5516E+04	0.0000E+00	0.5516E+04	0.5515E+04	
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231	GRS CALORI VALUE	0.0000E+00	0.1148E+05	0.0000E+00	0.1148E+05	0.1148E+05	
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232 -----

233

234 IDEAL GAS COMPOSITION (MOLAR BASE):

235

	impurities	dry_PG	USED FUEL	FLUE GAS	USED AIR	
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237 -----

238	HYDROGEN	0.0000E+00	0.2614E+00	0.3681E-01	0.0000E+00	0.0000E+00	
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239	OXYGEN	0.0000E+00	0.0000E+00	0.0000E+00	0.1528E+00	0.1817E+00	
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240	NITROGEN	0.0000E+00	0.2983E+00	0.2933E+00	0.7313E+00	0.7981E+00	
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241	CARBON MONOXIDE	0.0000E+00	0.1815E+00	0.2593E-01	0.0000E+00	0.0000E+00	
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242	CARBON DIOXIDE	0.0000E+00	0.1179E+00	0.2786E+00	0.4265E-01	0.3098E-03	
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243	WATER (I.G.)	0.0000E+00	0.1269E+00	0.3654E+00	0.6501E-01	0.1043E-01	
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244	HYDROGEN SULFIDE	0.1000E+01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
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245	METHANE	0.0000E+00	0.1042E-01	0.1321E-06	0.0000E+00	0.0000E+00	
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246	ARGON	0.0000E+00	0.3547E-02	0.0000E+00	0.8219E-02	0.9500E-02	
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247 -----

248	MEAN MOLE MASS	0.3408E+02	0.2175E+02	0.2786E+02	0.2875E+02	0.2875E+02	
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249	NET CALORI VALUE	0.1521E+05	0.5652E+04	0.5829E+03	0.0000E+00	0.0000E+00	
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250	GRS CALORI VALUE	0.1650E+05	0.1172E+05	0.2279E+04	0.0000E+00	0.0000E+00	
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251 -----

252

253 NON-IDEAL FLUID AND SOLID COMPOSITION (MASS BASE):

254

	Wood	DryWood	Ash	
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256 -----

257	HYDROGEN	0.4204E-01	0.5890E-01	0.0000E+00	
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258	OXYGEN	0.2976E+00	0.4171E+00	0.0000E+00	
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259	NITROGEN	0.1153E-02	0.1615E-02	0.0000E+00	
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260	CARBON (SOLID)	0.3309E+00	0.4636E+00	0.0000E+00	
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261	SULFUR (SOLID)	0.1356E-03	0.1900E-03	0.0000E+00	
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262	WATER (LIQUID)	0.3220E+00	0.5000E-01	0.0000E+00	
-----	----------------	------------	------------	------------	--

263	ASHES	0.6170E-02	0.8645E-02	0.1000E+01	
-----	-------	------------	------------	------------	--

264 -----

265	MEAN MOLE MASS	0.1321E+02	0.1193E+02	0.7600E+02	
-----	----------------	------------	------------	------------	--

266	NET CALORI VALUE	0.1161E+05	0.1724E+05	0.0000E+00	
-----	------------------	------------	------------	------------	--

267	GRS CALORI VALUE	0.1331E+05	0.1865E+05	0.0000E+00	
-----	------------------	------------	------------	------------	--

268 -----

DNA Output for SOFC–MGT scenario

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```
268
269
270 MEDIUM 97 : WATER FOR GAS APP
271 MEDIUM 300 : HEAT
272 MEDIUM 301 : PRODUCT HEAT
273
274
275 NUMBER OF CLOSED INTERNAL LOOPS IN THE SYSTEM:    0
276
277
278
279
280
281 SOLUTION FOR THE INDEPENDENT ALGEBRAIC VARIABLES :
282
283
284 VARIABLE NO | COMPONENT      | NAME      | VALUE |
285 -----
286      1 | Gasifier       | MULTIPLIER H | 0.8501E+05 |
287      2 | Gasifier       | MULTIPLIER C | 0.4364E+05 |
288      3 | Gasifier       | MULTIPLIER N | 0.1173E+06 |
289      4 | Gasifier       | MULTIPLIER O | 0.3125E+06 |
290      5 | Gasifier       | MULTIPLIER S | 0.1828E+06 |
291      6 | Gasifier       | MULTIPL Ar   | 0.2292E+06 |
292      7 | Gasifier       | GIBBS ENERGY | -.3280E+06 |
293      1 | airpreheat     | Transferred  | 0.3503E+02 |
294      1 | steamheater     | Transferred  | 0.3894E+02 |
295      1 | PGpreheat      | Transferred  | 0.6141E+02 |
296      1 | recuperator     | Transferred  | 0.2691E+03 |
297      1 | airpreheat2    | Transferred  | 0.9300E+02 |
298      1 | sofc           | MULTIPLIER H | 0.8954E+05 |
299      2 | sofc           | MULTIPLIER C | 0.7760E+05 |
300      3 | sofc           | MULTIPLIER N | 0.1131E+06 |
301      4 | sofc           | MULTIPLIER O | 0.2875E+06 |
302      5 | sofc           | GIBBS ENERGY | -.4347E+06 |
303      6 | sofc           | ETAMAX       | 0.7031E+00 |
304      7 | sofc           | ETASYS       | 0.8491E+00 |
305      8 | sofc           | UF           | 0.8500E+00 |
306      9 | sofc           | ETATOT       | 0.5074E+00 |
307     10 | sofc           | STCR         | 0.4098E+00 |
308     11 | sofc           | E_nernst     | 0.9653E+00 |
309     12 | sofc           | V_act        | 0.1081E+00 |
310     13 | sofc           | V_ohm        | 0.7147E-02 |
311     14 | sofc           | V_conc       | 0.3043E-01 |
312     15 | sofc           | V_cell       | 0.8196E+00 |
313     16 | sofc           | GMAX         | -.8644E+05 |
314     17 | sofc           | G(T)         | -.1885E+06 |
315     18 | sofc           | G(p,T)       | -.1863E+06 |
316     19 | sofc           | p_H2eq       | 0.6834E+00 |
317     20 | sofc           | R_e          | 0.2336E-01 |
318     21 | sofc           | Area [cm^2]  | 0.1013E+04 |
319     22 | sofc           | i_load       | 0.3000E+03 |
320     23 | sofc           | eta_DCAC     | 0.9500E+00 |
321      1 | burner         | Lambda       | 0.3600E+02 |
322      1 | exhaustcooler  | Transferred  | 0.1068E+03 |
```

```
322 -----
323 -----
324 -----
325 =====
326 #####
end
```

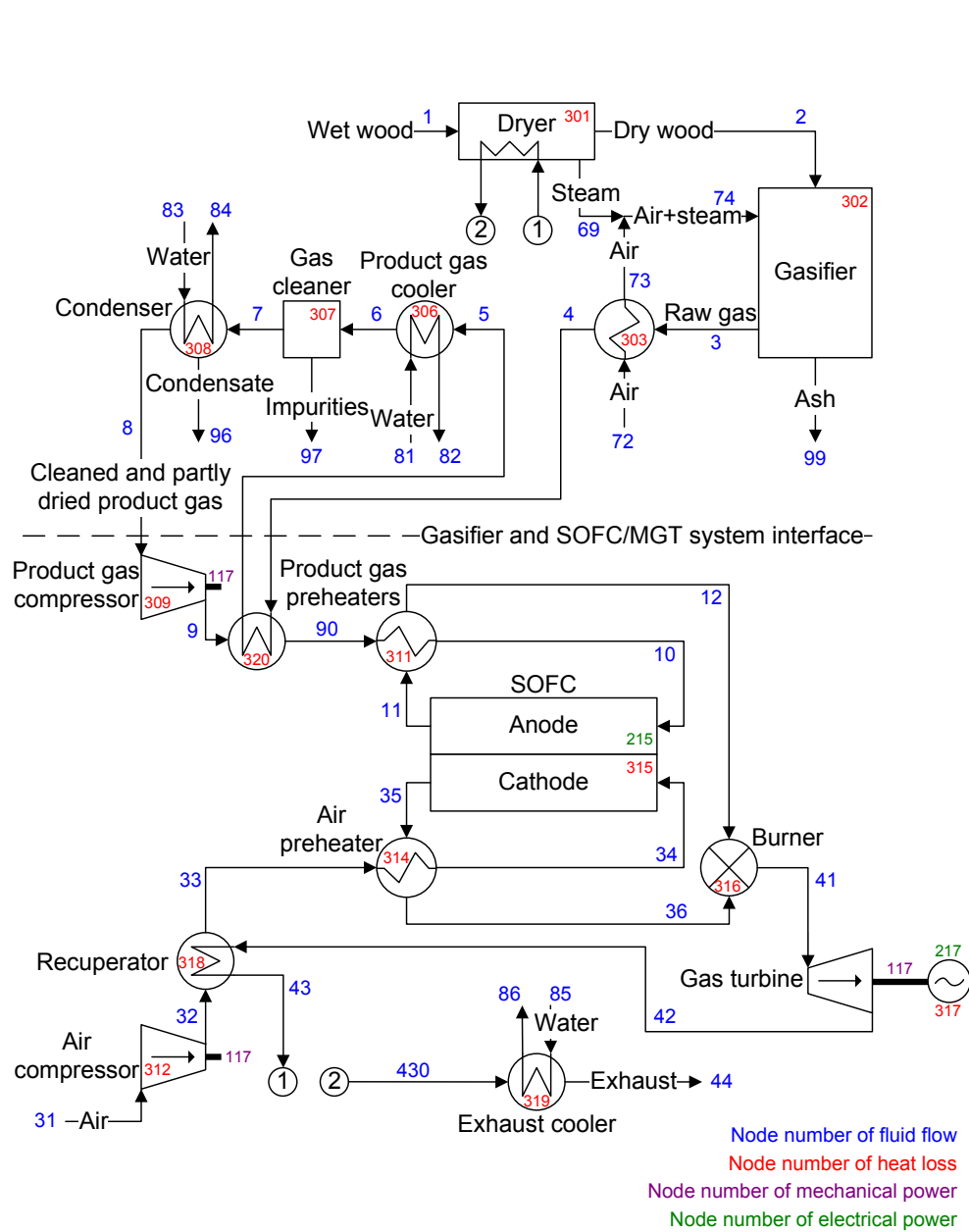
Appendix F OPTIMIZED SOFC-MGT PLANT MODEL LISTING

Included in this Appendix are:

- Flow sheet of optimized SOFC-MGT scenario with node numbers (1 page)
- DNA Input for optimized SOFC-MGT scenario (10 pages)
- DNA Output for optimized SOFC-MGT scenario (7 pages)

The input and output data only represent one simulation using the reference conditions.

Flow sheet of optimized SOFC-MGT scenario with node numbers



DNA Input for optimized SOFC-MGT scenario

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```
1 title Optimized Biomass gasification (Viking) + SOFC/MGT incl. recuperation
2 C Wood is dried and gasified. The gasification is atmospheric,
3 C based on air, and almost reaches equilibrium. The produced
4 C product gas (PG) composition and the cold gas efficiency is
5 C similar to that from the Viking gasifier.
6 C Power and heat production by a hybrid SOFC/MGT system.
7
8
9 C #####
10 C #####
11 C #####
12 C -----GASIFIER PART-----
13 C #####
14 C #####
15 C #####
16
17 C ##Media##
18 media 1 Wood 2 DryWood
19 media 73 STANDARD_AIR 3 raw_PG 99 Ash
20
21 C ##Fuel composition##
22 solid Wood C 0.488 H .062 O .439 S .0002 N 0.0017 ASH .0091
23 + LHV 18280 CP 1.35 MOI .322
24 C [Ahrenfeldt, J. et al., Energy & Fuels 2006, 20, 2672-2680] without Cl.
25
26
27
28 C #####
29 C -----DRYER-----
30 C #####
31 struc Dryer DRYER_03 1 64 2 61 301 0.05 0.005
32
33 C Fuel input (plant size):
34 addco m Dryer 1 0.043
35
36 addco t Dryer 1 15 p 1 1.013
37 addco p 2 1.008 t Dryer 2 150
38 addco q Dryer 301 0
39
40
41
42 C #####
43 C -----GASIFIER-----
44 C #####
45 struc Gasifier GASIFI_3 8 2 26 74 3 99 302 1 3 4 6 7 9 11 36 /
46 0.998 800 0.005 0 1.0 0.01
47 C Variable constitution parameter: Number of calculated gas components 8
48 C Nodes: Inlet fuel 2; inlet water 26; inlet air 74; outlet PG 3,
49 C outlet ash 99, heat loss 302
50 C Integer Parameters: Calculated gas compounds H2 (1), N2 (3), CO (4),
51 C CO2 (6), H2O (7), H2S (9), CH4 (11), Ar (36)
52 C Real parameter: Pressure 1 bar, Eq. temperature 800 degC, Pressure loss 0,
53 C Water-to-fuel ratio 0, carbon conversion factor 1,
54 C non-equilibrium methane 0.01.
55
56 addco t Gasifier 3 800
57 addco t Gasifier 26 150
58 addco p 99 1.013
59 addco q Gasifier 302 0
60
61
62
63 C #####
64 C -----GASIFIER AIR PREHEATER-----
65 C #####
66 struc airpreheat heatex_2 3 4 72 73 303 20 0.005 0.005
67 addco t airpreheat 72 15
68 addco q airpreheat 303 0
69
70
71
72 C #####
73 C -----STEAM HEATER-----
74 C #####
75 struc steamheater heatex_1 43 430 63 64 304 0.005 0.005
76
```

DNA Input for optimized SOFC-MGT scenario

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```
77 media 63 STEAM-HF
78
79 addco t steamheater 64 250
80 addco q steamheater 304 0
81
82
83
84 C #####
85 C -----STEAM BLOWER-----
86 C #####
87 struc steamblower COMPRE_1 61 62 305 105 0.6 0.98
88
89
90
91 C #####
92 C -----SPLITTER-----
93 C #####
94 struc split1 SPLITTER 62 63 69
95
96
97
98 C #####
99 C -----MIXER-----
100 C #####
101 struc mix1 MIXER_02 73 69 74
102
103 media 74 humid_air
104
105
106
107 C #####
108 C -----GAS COOLER-----
109 C #####
110 struc gascooler GASCOOL1 5 6 98 81 82 306 0.005 0.005
111
112 media 81 STEAM-HF 6 cold_PG
113
114 addco t gascooler 6 90
115 addco t gascooler 81 30 p 81 1.013
116 addco t gascooler 82 80
117 addco q gascooler 306 0
118
119
120
121 C #####
122 C -----GAS CLEANING-----
123 C #####
124 struc gasclean GASCLE_1 6 7 97 307 0.0049
125 C Pressure loss is taken from paper about Viking
126
127 media 7 clean_PG 97 impurities
128
129 addco q gasclean 307 0
130
131
132
133 C #####
134 C -----CONDENSER-----
135 C #####
136 struc condenser GASCOOL1 7 8 96 83 84 308 0.005 0.005
137
138 media 83 STEAM-HF 8 dry_PG
139
140 addco t condenser 8 50
141 addco t condenser 83 30 p 83 1.013
142 addco t condenser 84 80
143 addco q condenser 308 0
144
145
146
147 C #####
148 C #####
149 C #####
150 C -----SOFC PART-----
151 C #####
152 C #####
```

DNA Input for optimized SOFC-MGT scenario

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```
153 C #####
154
155 media 11 USED FUEL 35 USED AIR
156
157
158
159 C #####
160 C -----PRODUCT GAS COMPRESSOR-----
161 C #####
162 struc PGcompressor compre_1 8 9 309 117 0.75 0.98
163 C Isentropic efficiency from L. Fryda et al. (2008)
164
165
166
167 C #####
168 C -----FIRST STEP PRODUCT GAS PREHEATING-----
169 C #####
170 struc PGpreheat0 heatex_4 4 5 9 90 320 0.85 0.005 0.005
171 addco q PGpreheat0 320 0
172
173
174
175 C #####
176 C -----SECOND STEP PRODUCT GAS PREHEATING-----
177 C #####
178 struc PGpreheat heatex_2 11 12 90 10 311 150 0.005 0.005
179 addco q PGpreheat 311 0
180
181
182
183 C #####
184 C -----AIR COMPRESSOR-----
185 C #####
186 struc aircompressor compre_1 31 32 312 117 0.75 0.98
187 C Isentropic efficiency from L. Fryda et al. (2008)
188
189 media 31 STANDARD_AIR
190 addco p 31 1.013 t aircompressor 31 15
191
192
193
194 C #####
195 C -----RECUPERATOR-----
196 C #####
197 struc recuperator heatex_4 42 43 32 33 318 0.85 0.01 0.01
198 addco q recuperator 318 0
199
200
201
202 C #####
203 C -----SOFC AIR PREHEATING-----
204 C #####
205 struc airpreheat2 heatex_2 35 36 33 34 314 200 0.01 0.01
206 addco q airpreheat2 314 0
207
208
209
210 C #####
211 C -----SOFC-----
212 C #####
213 struc sofc sofceq0d_CBM /
214 {fuel and air inlets} 10 34 /
215 {fuel and air outlets} 11 35 /
216 {nodes for power and heat loss} 215 315 /
217 {parameters: utilization, temperature} 0.85 800 /
218 {pressure loss} 0.005 0.010 /
219 {temperature difference between anode and cathode outlet} 0 /
220 {current density [mA/cm^2]} 300 /
221 {DC to AC conversion efficiency [-]} 0.95
222
223 addco q sofc 315 0
224
225 C SOFC OPERATING PRESSURE:
226 addco p 10 2.75
227
228
```

```

229
230 C #####
231 C -----BURNER-----
232 C #####
233 struc burner GASBUR_3 36 12 41 316 0.999374
234
235 media 41 FLUE_GAS
236
237 addco q burner 316 0
238
239
240
241 C #####
242 C -----GAS TURBINE-----
243 C #####
244 struc GT turbin_1 41 42 117 0.84
245 C Isentropic efficiency from L. Fryda et al. (2008)
246
247
248
249 C #####
250 C -----GENERATOR-----
251 C #####
252 struc generator sim_gene 217 317 117 0.95
253
254
255
256 C #####
257 C -----EXHAUST COOLING-----
258 C #####
259 struc exhaustcooler heatex_2 430 44 85 86 319 60 0.010 0.005
260
261 media 85 STEAM-HF
262
263 addco p 44 1.013
264 addco p 85 1.013 t exhaustcooler 85 30
265 addco t exhaustcooler 86 80
266 addco q exhaustcooler 319 0
267
268
269
270 C Reference conditions for exergy
271 xergy p 1 t 15
272
273
274
275
276
277 C ~~~~~
~~~~~
278 C ~~ Start of list of generated initial guesses.
279 C ~~ The values are the results of the latest simulation.
280 C ~~~~~
~~~~~
281 START M      Dryer      1  0.43000000000000001E-01 {~~}
282 START P      1  0.10130000000000000E+01 {~~}
283 START H      Dryer      1  -0.8621618755529536E+04 {~~}
284 START M      Dryer      64  0.2000459030657078E+00 {~~}
285 START P      64  0.99800000000000002E+00 {~~}
286 START H      Dryer      64  -0.1299653551379773E+05 {~~}
287 START M      Dryer      2  -0.3068842105263158E-01 {~~}
288 START P      2  0.10080000000000000E+01 {~~}
289 START H      Dryer      2  -0.5497059220211002E+04 {~~}
290 START M      Dryer      61  -0.2123574820130763E+00 {~~}
291 START P      61  0.99300000000000002E+00 {~~}
292 START H      Dryer      61  -0.1319443607829820E+05 {~~}
293 START Q      Dryer      301  0.00000000000000000E+00 {~~}
294 START X_J    DryWood    H2      0.589000000000000001E-01 {~~}
295 START X_J    DryWood    O2      0.417050000000000001E+00 {~~}
296 START X_J    DryWood    N2      0.16150000000000000E-02 {~~}
297 START X_J    DryWood    CO      0.00000000000000000E+00 {~~}
298 START X_J    DryWood    NO      0.00000000000000000E+00 {~~}
299 START X_J    DryWood    CO2     0.00000000000000000E+00 {~~}
300 START X_J    DryWood    H2O-L   0.50000000000000000E-01 {~~}
301 START X_J    DryWood    NH3     0.00000000000000000E+00 {~~}
302 START X_J    DryWood    H2S     0.00000000000000000E+00 {~~}

```

DNA Input for optimized SOFC-MGT scenario

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303	START X_J	DryWood	SO2	0.0000000000000000E+00	{~~}
304	START X_J	DryWood	CH4	0.0000000000000000E+00	{~~}
305	START X_J	DryWood	C2H6	0.0000000000000000E+00	{~~}
306	START X_J	DryWood	C3H8	0.0000000000000000E+00	{~~}
307	START X_J	DryWood	C4H10-N	0.0000000000000000E+00	{~~}
308	START X_J	DryWood	C4H10-I	0.0000000000000000E+00	{~~}
309	START X_J	DryWood	C5H12	0.0000000000000000E+00	{~~}
310	START X_J	DryWood	C6H14	0.0000000000000000E+00	{~~}
311	START X_J	DryWood	C7H16	0.0000000000000000E+00	{~~}
312	START X_J	DryWood	C8H18	0.0000000000000000E+00	{~~}
313	START X_J	DryWood	C2H4	0.0000000000000000E+00	{~~}
314	START X_J	DryWood	C3H6	0.0000000000000000E+00	{~~}
315	START X_J	DryWood	C5H10	0.0000000000000000E+00	{~~}
316	START X_J	DryWood	C6H12-1	0.0000000000000000E+00	{~~}
317	START X_J	DryWood	C7H14	0.0000000000000000E+00	{~~}
318	START X_J	DryWood	C2H2	0.0000000000000000E+00	{~~}
319	START X_J	DryWood	C6H6	0.0000000000000000E+00	{~~}
320	START X_J	DryWood	C6H12-C	0.0000000000000000E+00	{~~}
321	START X_J	DryWood	C	0.4636000000000001E+00	{~~}
322	START X_J	DryWood	S	0.1900000000000000E-03	{~~}
323	START X_J	DryWood	NO2	0.0000000000000000E+00	{~~}
324	START X_J	DryWood	HCN	0.0000000000000000E+00	{~~}
325	START X_J	DryWood	COS	0.0000000000000000E+00	{~~}
326	START X_J	DryWood	N2O	0.0000000000000000E+00	{~~}
327	START X_J	DryWood	NO3	0.0000000000000000E+00	{~~}
328	START X_J	DryWood	SO3	0.0000000000000000E+00	{~~}
329	START X_J	DryWood	AR	0.0000000000000000E+00	{~~}
330	START X_J	DryWood	ASH	0.8645000000000003E-02	{~~}
331	START X_J	DryWood	TAR	0.0000000000000000E+00	{~~}
332	START M	Gasifier	2	0.3068842105263158E-01	{~~}
333	START H	Gasifier	2	-0.5497059220211002E+04	{~~}
334	START M	Gasifier	26	0.0000000000000000E+00	{~~}
335	START P		26	0.1003000000000000E+01	{~~}
336	START H	Gasifier	26	-0.1319450918722706E+05	{~~}
337	START M	Gasifier	74	0.5485206982616295E-01	{~~}
338	START P		74	0.1003000000000000E+01	{~~}
339	START H	Gasifier	74	-0.2398848478333933E+04	{~~}
340	START M	Gasifier	3	-0.8527518947879453E-01	{~~}
341	START P		3	0.9980000000000002E+00	{~~}
342	START H	Gasifier	3	-0.3507877913073764E+04	{~~}
343	START M	Gasifier	99	-0.2653014000000001E-03	{~~}
344	START P		99	0.1013000000000000E+01	{~~}
345	START H	Gasifier	99	-0.4307999999999999E+04	{~~}
346	START Q	Gasifier	302	0.0000000000000000E+00	{~~}
347	START ZA	Gasifier	1	0.8500945239865246E+05	{~~}
348	START ZA	Gasifier	2	0.4363965291425175E+05	{~~}
349	START ZA	Gasifier	3	0.1172765217993686E+06	{~~}
350	START ZA	Gasifier	4	0.3124902840469573E+06	{~~}
351	START ZA	Gasifier	5	0.1827651987487788E+06	{~~}
352	START ZA	Gasifier	6	0.2292482774424771E+06	{~~}
353	START ZA	Gasifier	7	-0.3279719879436734E+06	{~~}
354	START Y_J	raw_PG	H2	0.2538114658675973E+00	{~~}
355	START Y_J	raw_PG	O2	0.0000000000000000E+00	{~~}
356	START Y_J	raw_PG	N2	0.2896541868376537E+00	{~~}
357	START Y_J	raw_PG	CO	0.1761818347160896E+00	{~~}
358	START Y_J	raw_PG	NO	0.0000000000000000E+00	{~~}
359	START Y_J	raw_PG	CO2	0.1144395150133744E+00	{~~}
360	START Y_J	raw_PG	H2O-G	0.1523098114753785E+00	{~~}
361	START Y_J	raw_PG	NH3	0.0000000000000000E+00	{~~}
362	START Y_J	raw_PG	H2S	0.4615796164902303E-04	{~~}
363	START Y_J	raw_PG	SO2	0.0000000000000000E+00	{~~}
364	START Y_J	raw_PG	CH4	0.1011293223314738E-01	{~~}
365	START Y_J	raw_PG	NO2	0.0000000000000000E+00	{~~}
366	START Y_J	raw_PG	HCN	0.0000000000000000E+00	{~~}
367	START Y_J	raw_PG	COS	0.0000000000000000E+00	{~~}
368	START Y_J	raw_PG	AR	0.3444095895110029E-02	{~~}
369	START X_J	Ash	C	0.0000000000000000E+00	{~~}
370	START X_J	Ash	ASH	0.1000000000000000E+01	{~~}
371	START M	airpreheat	3	0.8527518947879453E-01	{~~}
372	START H	airpreheat	3	-0.3507877913073763E+04	{~~}
373	START M	airpreheat	4	-0.8527518947879453E-01	{~~}
374	START P		4	0.9930000000000002E+00	{~~}
375	START H	airpreheat	4	-0.3918630307677496E+04	{~~}
376	START M	airpreheat	72	0.4254049087879453E-01	{~~}
377	START P		72	0.1008000000000000E+01	{~~}
378	START H	airpreheat	72	-0.9883454496688232E+02	{~~}

DNA Input for optimized SOFC-MGT scenario

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379	START M	airpreheat	73	-0.4254049087879453E-01	{~~}
380	START P		73	0.1003000000000000E+01	{~~}
381	START H	airpreheat	73	0.7245454291500130E+03	{~~}
382	START Q	airpreheat	303	0.0000000000000000E+00	{~~}
383	START ZA	airpreheat	1	0.3502698827870186E+02	{~~}
384	START M	steamheater	43	0.8013142818653432E+00	{~~}
385	START P		43	0.1028000000000000E+01	{~~}
386	START H	steamheater	43	-0.8735921928420305E+03	{~~}
387	START M	steamheater	430	-0.8013142818653432E+00	{~~}
388	START P		430	0.1023000000000000E+01	{~~}
389	START H	steamheater	430	-0.9221860411687504E+03	{~~}
390	START M	steamheater	63	0.2000459030657078E+00	{~~}
391	START P		63	0.1003000000000000E+01	{~~}
392	START H	steamheater	63	-0.1319118556200296E+05	{~~}
393	START M	steamheater	64	-0.2000459030657078E+00	{~~}
394	START H	steamheater	64	-0.1299653551379773E+05	{~~}
395	START Q	steamheater	304	0.0000000000000000E+00	{~~}
396	START ZA	steamheater	1	0.3893894467499903E+02	{~~}
397	START M	steamblower	61	0.2123574820130763E+00	{~~}
398	START H	steamblower	61	-0.1319443607829820E+05	{~~}
399	START M	steamblower	62	-0.2123574820130763E+00	{~~}
400	START P		62	0.1003000000000000E+01	{~~}
401	START H	steamblower	62	-0.1319118556200296E+05	{~~}
402	START Q	steamblower	305	-0.1408717256529214E-01	{~~}
403	START W	steamblower	105	0.7043586282646008E+00	{~~}
404	START M	split1	62	0.2123574820130763E+00	{~~}
405	START H	split1	62	-0.1319118556200296E+05	{~~}
406	START M	split1	63	-0.2000459030657078E+00	{~~}
407	START H	split1	63	-0.1319118556200296E+05	{~~}
408	START M	split1	69	-0.1231157894736842E-01	{~~}
409	START P		69	0.1003000000000000E+01	{~~}
410	START H	split1	69	-0.1319118556200296E+05	{~~}
411	START M	mix1	73	0.4254049087879453E-01	{~~}
412	START H	mix1	73	0.7245454291500130E+03	{~~}
413	START M	mix1	69	0.1231157894736842E-01	{~~}
414	START H	mix1	69	-0.1319118556200297E+05	{~~}
415	START M	mix1	74	-0.5485206982616295E-01	{~~}
416	START H	mix1	74	-0.2398848478333933E+04	{~~}
417	START Y_J	humid_air	H2	0.0000000000000000E+00	{~~}
418	START Y_J	humid_air	O2	0.1417803964772675E+00	{~~}
419	START Y_J	humid_air	N2	0.5281063539146027E+00	{~~}
420	START Y_J	humid_air	CO	0.0000000000000000E+00	{~~}
421	START Y_J	humid_air	NO	0.0000000000000000E+00	{~~}
422	START Y_J	humid_air	CO2	0.2049837057502663E-03	{~~}
423	START Y_J	humid_air	H2O-G	0.3236220989260379E+00	{~~}
424	START Y_J	humid_air	NH3	0.0000000000000000E+00	{~~}
425	START Y_J	humid_air	H2S	0.0000000000000000E+00	{~~}
426	START Y_J	humid_air	SO2	0.0000000000000000E+00	{~~}
427	START Y_J	humid_air	CH4	0.0000000000000000E+00	{~~}
428	START Y_J	humid_air	C2H6	0.0000000000000000E+00	{~~}
429	START Y_J	humid_air	C3H8	0.0000000000000000E+00	{~~}
430	START Y_J	humid_air	C4H10-N	0.0000000000000000E+00	{~~}
431	START Y_J	humid_air	C4H10-I	0.0000000000000000E+00	{~~}
432	START Y_J	humid_air	C5H12	0.0000000000000000E+00	{~~}
433	START Y_J	humid_air	C6H14	0.0000000000000000E+00	{~~}
434	START Y_J	humid_air	C7H16	0.0000000000000000E+00	{~~}
435	START Y_J	humid_air	C8H18	0.0000000000000000E+00	{~~}
436	START Y_J	humid_air	C2H4	0.0000000000000000E+00	{~~}
437	START Y_J	humid_air	C3H6	0.0000000000000000E+00	{~~}
438	START Y_J	humid_air	C5H10	0.0000000000000000E+00	{~~}
439	START Y_J	humid_air	C6H12-1	0.0000000000000000E+00	{~~}
440	START Y_J	humid_air	C7H14	0.0000000000000000E+00	{~~}
441	START Y_J	humid_air	C2H2	0.0000000000000000E+00	{~~}
442	START Y_J	humid_air	C6H6	0.0000000000000000E+00	{~~}
443	START Y_J	humid_air	C6H12-C	0.0000000000000000E+00	{~~}
444	START Y_J	humid_air	C	0.0000000000000000E+00	{~~}
445	START Y_J	humid_air	S	0.0000000000000000E+00	{~~}
446	START Y_J	humid_air	NO2	0.0000000000000000E+00	{~~}
447	START Y_J	humid_air	HCN	0.0000000000000000E+00	{~~}
448	START Y_J	humid_air	COS	0.0000000000000000E+00	{~~}
449	START Y_J	humid_air	N2O	0.0000000000000000E+00	{~~}
450	START Y_J	humid_air	NO3	0.0000000000000000E+00	{~~}
451	START Y_J	humid_air	SO3	0.0000000000000000E+00	{~~}
452	START Y_J	humid_air	AR	0.6286166976341500E-02	{~~}
453	START Y_J	humid_air	ASH	0.0000000000000000E+00	{~~}
454	START Y_J	humid_air	TAR	0.0000000000000000E+00	{~~}

DNA Input for optimized SOFC-MGT scenario

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455 START Y_J humid_air CH3OH 0.0000000000000000E+00 {~~}
456 START M_ gascooler 5 0.8527518947879453E-01 {~~}
457 START P 5 0.9880000000000000E+00 {~~}
458 START H gascooler 5 -0.4379339392033765E+04 {~~}
459 START M gascooler 6 -0.8527518947879453E-01 {~~}
460 START P 6 0.9830000000000000E+00 {~~}
461 START H gascooler 6 -0.4624611248324029E+04 {~~}
462 START M gascooler 98 0.0000000000000000E+00 {~~}
463 START P 98 0.9830000000000000E+00 {~~}
464 START H gascooler 98 -0.1559408877861425E+05 {~~}
465 START M gascooler 81 0.9999930726503181E-01 {~~}
466 START P 81 0.1013000000000000E+01 {~~}
467 START H gascooler 81 -0.1584524528596511E+05 {~~}
468 START M gascooler 82 -0.9999930726503181E-01 {~~}
469 START P 82 0.1008000000000000E+01 {~~}
470 START H gascooler 82 -0.1563608779686837E+05 {~~}
471 START Q gascooler 306 0.0000000000000000E+00 {~~}
472 START Y_J cold_PG H2 0.2538114658675976E+00 {~~}
473 START Y_J cold_PG O2 0.0000000000000000E+00 {~~}
474 START Y_J cold_PG N2 0.2896541868376540E+00 {~~}
475 START Y_J cold_PG CO 0.1761818347160898E+00 {~~}
476 START Y_J cold_PG NO 0.0000000000000000E+00 {~~}
477 START Y_J cold_PG CO2 0.1144395150133745E+00 {~~}
478 START Y_J cold_PG H2O-G 0.1523098114753785E+00 {~~}
479 START Y_J cold_PG NH3 0.0000000000000000E+00 {~~}
480 START Y_J cold_PG H2S 0.4615796164902308E-04 {~~}
481 START Y_J cold_PG SO2 0.0000000000000000E+00 {~~}
482 START Y_J cold_PG CH4 0.1011293223314739E-01 {~~}
483 START Y_J cold_PG C2H6 0.0000000000000000E+00 {~~}
484 START Y_J cold_PG C3H8 0.0000000000000000E+00 {~~}
485 START Y_J cold_PG C4H10-N 0.0000000000000000E+00 {~~}
486 START Y_J cold_PG C4H10-I 0.0000000000000000E+00 {~~}
487 START Y_J cold_PG C5H12 0.0000000000000000E+00 {~~}
488 START Y_J cold_PG C6H14 0.0000000000000000E+00 {~~}
489 START Y_J cold_PG C7H16 0.0000000000000000E+00 {~~}
490 START Y_J cold_PG C8H18 0.0000000000000000E+00 {~~}
491 START Y_J cold_PG C2H4 0.0000000000000000E+00 {~~}
492 START Y_J cold_PG C3H6 0.0000000000000000E+00 {~~}
493 START Y_J cold_PG C5H10 0.0000000000000000E+00 {~~}
494 START Y_J cold_PG C6H12-1 0.0000000000000000E+00 {~~}
495 START Y_J cold_PG C7H14 0.0000000000000000E+00 {~~}
496 START Y_J cold_PG C2H2 0.0000000000000000E+00 {~~}
497 START Y_J cold_PG C6H6 0.0000000000000000E+00 {~~}
498 START Y_J cold_PG C6H12-C 0.0000000000000000E+00 {~~}
499 START Y_J cold_PG C 0.0000000000000000E+00 {~~}
500 START Y_J cold_PG S 0.0000000000000000E+00 {~~}
501 START Y_J cold_PG NO2 0.0000000000000000E+00 {~~}
502 START Y_J cold_PG HCN 0.0000000000000000E+00 {~~}
503 START Y_J cold_PG COS 0.0000000000000000E+00 {~~}
504 START Y_J cold_PG N2O 0.0000000000000000E+00 {~~}
505 START Y_J cold_PG NO3 0.0000000000000000E+00 {~~}
506 START Y_J cold_PG SO3 0.0000000000000000E+00 {~~}
507 START Y_J cold_PG AR 0.3444095895110033E-02 {~~}
508 START M gasclean 6 0.8527518947879453E-01 {~~}
509 START H gasclean 6 -0.4624611248324028E+04 {~~}
510 START M gasclean 7 -0.8526899202586877E-01 {~~}
511 START P 7 0.9781000000000000E+00 {~~}
512 START H gasclean 7 -0.4624908439609411E+04 {~~}
513 START M gasclean 97 -0.6197452925764196E-05 {~~}
514 START P 97 0.9781000000000000E+00 {~~}
515 START H gasclean 97 -0.5356408846834924E+03 {~~}
516 START Q gasclean 307 0.0000000000000000E+00 {~~}
517 START Y_J clean_PG H2 0.2538231818282898E+00 {~~}
518 START Y_J clean_PG O2 0.0000000000000000E+00 {~~}
519 START Y_J clean_PG N2 0.2896675573016547E+00 {~~}
520 START Y_J clean_PG CO 0.1761899672858426E+00 {~~}
521 START Y_J clean_PG NO 0.0000000000000000E+00 {~~}
522 START Y_J clean_PG CO2 0.1144447975519507E+00 {~~}
523 START Y_J clean_PG H2O-G 0.1523168421103350E+00 {~~}
524 START Y_J clean_PG CH4 0.1011339904703273E-01 {~~}
525 START Y_J clean_PG NO2 0.0000000000000000E+00 {~~}
526 START Y_J clean_PG AR 0.3444254874894455E-02 {~~}
527 START Y_J impurities H2O-G 0.0000000000000000E+00 {~~}
528 START Y_J impurities NH3 0.0000000000000000E+00 {~~}
529 START Y_J impurities H2S 0.1000000000000000E+01 {~~}
530 START Y_J impurities SO2 0.0000000000000000E+00 {~~}

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DNA Input for optimized SOFC-MGT scenario

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531	START Y_J	impurities	HCN	0.0000000000000000E+00	{~~}
532	START Y_J	impurities	COS	0.0000000000000000E+00	{~~}
533	START Y_J	impurities	AR	0.0000000000000000E+00	{~~}
534	START Y_J	impurities	ASH	0.0000000000000000E+00	{~~}
535	START M	condenser	7	0.8526899202586877E-01	{~~}
536	START H	condenser	7	-0.4624908439609411E+04	{~~}
537	START M	condenser	8	-0.8320484335731894E-01	{~~}
538	START P		8	0.9731000000000002E+00	{~~}
539	START H	condenser	8	-0.4466561290262755E+04	{~~}
540	START M	condenser	96	-0.2064148668549822E-02	{~~}
541	START P		96	0.9731000000000002E+00	{~~}
542	START H	condenser	96	-0.1576166949955454E+05	{~~}
543	START M	condenser	83	0.4691527326491256E-01	{~~}
544	START P		83	0.1013000000000000E+01	{~~}
545	START H	condenser	83	-0.1584524528596511E+05	{~~}
546	START M	condenser	84	-0.4691527326491256E-01	{~~}
547	START P		84	0.1008000000000000E+01	{~~}
548	START H	condenser	84	-0.1563608779686837E+05	{~~}
549	START Q	condenser	308	0.0000000000000000E+00	{~~}
550	START Y_J	dry_PG	H2	0.2614256920940565E+00	{~~}
551	START Y_J	dry_PG	O2	0.0000000000000000E+00	{~~}
552	START Y_J	dry_PG	N2	0.2983436780648683E+00	{~~}
553	START Y_J	dry_PG	CO	0.1814672080223560E+00	{~~}
554	START Y_J	dry_PG	NO	0.0000000000000000E+00	{~~}
555	START Y_J	dry_PG	CO2	0.1178726473723855E+00	{~~}
556	START Y_J	dry_PG	H2O-G	0.1269270417636784E+00	{~~}
557	START Y_J	dry_PG	NH3	0.0000000000000000E+00	{~~}
558	START Y_J	dry_PG	H2S	0.0000000000000000E+00	{~~}
559	START Y_J	dry_PG	SO2	0.0000000000000000E+00	{~~}
560	START Y_J	dry_PG	CH4	0.1041631550849635E-01	{~~}
561	START Y_J	dry_PG	C2H6	0.0000000000000000E+00	{~~}
562	START Y_J	dry_PG	C3H8	0.0000000000000000E+00	{~~}
563	START Y_J	dry_PG	C4H10-N	0.0000000000000000E+00	{~~}
564	START Y_J	dry_PG	C4H10-I	0.0000000000000000E+00	{~~}
565	START Y_J	dry_PG	C5H12	0.0000000000000000E+00	{~~}
566	START Y_J	dry_PG	C6H14	0.0000000000000000E+00	{~~}
567	START Y_J	dry_PG	C7H16	0.0000000000000000E+00	{~~}
568	START Y_J	dry_PG	C8H18	0.0000000000000000E+00	{~~}
569	START Y_J	dry_PG	C2H4	0.0000000000000000E+00	{~~}
570	START Y_J	dry_PG	C3H6	0.0000000000000000E+00	{~~}
571	START Y_J	dry_PG	C5H10	0.0000000000000000E+00	{~~}
572	START Y_J	dry_PG	C6H12-1	0.0000000000000000E+00	{~~}
573	START Y_J	dry_PG	C7H14	0.0000000000000000E+00	{~~}
574	START Y_J	dry_PG	C2H2	0.0000000000000000E+00	{~~}
575	START Y_J	dry_PG	C6H6	0.0000000000000000E+00	{~~}
576	START Y_J	dry_PG	C6H12-C	0.0000000000000000E+00	{~~}
577	START Y_J	dry_PG	C	0.0000000000000000E+00	{~~}
578	START Y_J	dry_PG	S	0.0000000000000000E+00	{~~}
579	START Y_J	dry_PG	NO2	0.0000000000000000E+00	{~~}
580	START Y_J	dry_PG	HCN	0.0000000000000000E+00	{~~}
581	START Y_J	dry_PG	COS	0.0000000000000000E+00	{~~}
582	START Y_J	dry_PG	N2O	0.0000000000000000E+00	{~~}
583	START Y_J	dry_PG	NO3	0.0000000000000000E+00	{~~}
584	START Y_J	dry_PG	SO3	0.0000000000000000E+00	{~~}
585	START Y_J	dry_PG	AR	0.3547417174159995E-02	{~~}
586	START M	PGcompressor	8	0.8320484335731894E-01	{~~}
587	START H	PGcompressor	8	-0.4466561290262755E+04	{~~}
588	START M	PGcompressor	9	-0.8320484335731894E-01	{~~}
589	START P		9	0.2760000000000000E+01	{~~}
590	START H	PGcompressor	9	-0.4268497982768156E+04	{~~}
591	START Q	PGcompressor	309	-0.3363229892840937E+00	{~~}
592	START W	PGcompressor	117	0.1681614946420476E+02	{~~}
593	START M	PGpreheat0	4	0.8527518947879453E-01	{~~}
594	START H	PGpreheat0	4	-0.3918630307677496E+04	{~~}
595	START M	PGpreheat0	5	-0.8527518947879453E-01	{~~}
596	START H	PGpreheat0	5	-0.4379339392033766E+04	{~~}
597	START M	PGpreheat0	9	0.8320484335731894E-01	{~~}
598	START H	PGpreheat0	9	-0.4268497982768156E+04	{~~}
599	START M	PGpreheat0	90	-0.8320484335731894E-01	{~~}
600	START P		90	0.2755000000000000E+01	{~~}
601	START H	PGpreheat0	90	-0.3796325295724367E+04	{~~}
602	START Q	PGpreheat0	320	0.0000000000000000E+00	{~~}
603	START ZA	PGpreheat0	1	0.3928705446308283E+02	{~~}
604	START M	PGpreheat	11	0.1084136464468040E+00	{~~}
605	START P		11	0.2745000000000000E+01	{~~}
606	START H	PGpreheat	11	-0.6150751178803807E+04	{~~}

DNA Input for optimized SOFC-MGT scenario

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607	START M	PGpreheat	12	-0.1084136464468040E+00	{~~}
608	START P		12	0.2740000000000000E+01	{~~}
609	START H	PGpreheat	12	-0.6338869655258502E+04	{~~}
610	START M	PGpreheat	90	0.8320484335731894E-01	{~~}
611	START H	PGpreheat	90	-0.3796325295724366E+04	{~~}
612	START M	PGpreheat	10	-0.8320484335731894E-01	{~~}
613	START P		10	0.2750000000000000E+01	{~~}
614	START H	PGpreheat	10	-0.3551212040611476E+04	{~~}
615	START Q	PGpreheat	311	0.0000000000000000E+00	{~~}
616	START ZA	PGpreheat	1	0.2039460999647063E+02	{~~}
617	START M	aircompressor	31	0.7181094385080242E+00	{~~}
618	START P		31	0.1013000000000000E+01	{~~}
619	START H	aircompressor	31	-0.9883454496688232E+02	{~~}
620	START M	aircompressor	32	-0.7181094385080242E+00	{~~}
621	START P		32	0.2780000000000000E+01	{~~}
622	START H	aircompressor	32	0.3066441581850383E+02	{~~}
623	START Q	aircompressor	312	-0.1897845428917670E+01	{~~}
624	START W	aircompressor	117	0.9489227144588396E+02	{~~}
625	START M	airpreheat2	35	0.6929006354185392E+00	{~~}
626	START P		35	0.2750000000000000E+01	{~~}
627	START H	airpreheat2	35	0.7462226485113632E+03	{~~}
628	START M	airpreheat2	36	-0.6929006354185392E+00	{~~}
629	START P		36	0.2740000000000000E+01	{~~}
630	START H	airpreheat2	36	0.6693894914039743E+03	{~~}
631	START M	airpreheat2	33	0.7181094385080242E+00	{~~}
632	START P		33	0.2770000000000000E+01	{~~}
633	START H	airpreheat2	33	0.4452705848535890E+03	{~~}
634	START M	airpreheat2	34	-0.7181094385080242E+00	{~~}
635	START P		34	0.2760000000000000E+01	{~~}
636	START H	airpreheat2	34	0.5194065598541840E+03	{~~}
637	START Q	airpreheat2	314	0.0000000000000000E+00	{~~}
638	START ZA	airpreheat2	1	0.5323774338092223E+02	{~~}
639	START M	sofc	10	0.8320484335731894E-01	{~~}
640	START H	sofc	10	-0.3551212040611476E+04	{~~}
641	START M	sofc	34	0.7181094385080242E+00	{~~}
642	START H	sofc	34	0.5194065598541839E+03	{~~}
643	START M	sofc	11	-0.1084136464468040E+00	{~~}
644	START H	sofc	11	-0.6150751178803807E+04	{~~}
645	START M	sofc	35	-0.6929006354185392E+00	{~~}
646	START H	sofc	35	0.7462226485113632E+03	{~~}
647	START E	sofc	215	-0.2272799278504398E+03	{~~}
648	START Q	sofc	315	0.0000000000000000E+00	{~~}
649	START ZA	sofc	1	0.8910905268625762E+05	{~~}
650	START ZA	sofc	2	0.7674420988740612E+05	{~~}
651	START ZA	sofc	3	0.1127074608890391E+06	{~~}
652	START ZA	sofc	4	0.2874557230368785E+06	{~~}
653	START ZA	sofc	5	-0.4338076091026879E+06	{~~}
654	START ZA	sofc	6	0.7046466791463556E+00	{~~}
655	START ZA	sofc	7	0.8493901070235544E+00	{~~}
656	START ZA	sofc	8	0.8500000000000001E+00	{~~}
657	START ZA	sofc	9	0.5087419304818280E+00	{~~}
658	START ZA	sofc	10	0.4097643685146409E+00	{~~}
659	START ZA	sofc	11	0.9675017630887374E+00	{~~}
660	START ZA	sofc	12	0.1081415052915717E+00	{~~}
661	START ZA	sofc	13	0.7147434745365779E-02	{~~}
662	START ZA	sofc	14	0.3042639695637969E-01	{~~}
663	START ZA	sofc	15	0.8217864260954202E+00	{~~}
664	START ZA	sofc	16	-0.8662243293325575E+05	{~~}
665	START ZA	sofc	17	-0.1885369880714480E+06	{~~}
666	START ZA	sofc	18	-0.1866988152232337E+06	{~~}
667	START ZA	sofc	19	0.7518497376280033E+00	{~~}
668	START ZA	sofc	20	0.2335762988681627E-01	{~~}
669	START ZA	sofc	21	0.1013478073726872E+04	{~~}
670	START ZA	sofc	22	0.3000000000000000E+03	{~~}
671	START ZA	sofc	23	0.9500000000000001E+00	{~~}
672	START Y_J	USED FUEL	H2	0.3681256970852961E-01	{~~}
673	START Y_J	USED FUEL	CO	0.2592598083526594E-01	{~~}
674	START Y_J	USED FUEL	CO2	0.2785669018789887E+00	{~~}
675	START Y_J	USED FUEL	H2O-G	0.3654199260118688E+00	{~~}
676	START Y_J	USED FUEL	CH4	0.1598843230450034E-06	{~~}
677	START Y_J	USED FUEL	N2	0.2932744616810239E+00	{~~}
678	START Y_J	USED AIR	O2	0.1815942842608005E+00	{~~}
679	START Y_J	USED AIR	N2	0.7981650191732836E+00	{~~}
680	START Y_J	USED AIR	CO2	0.3098065800905487E-03	{~~}
681	START Y_J	USED AIR	H2O-G	0.1043015486304847E-01	{~~}
682	START Y_J	USED AIR	AR	0.9500735122776839E-02	{~~}

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683 START M burner 36 0.6929006354185392E+00 {~~}
684 START H burner 36 0.6693894914039743E+03 {~~}
685 START M burner 12 0.1084136464468040E+00 {~~}
686 START H burner 12 -0.6338869655258501E+04 {~~}
687 START M burner 41 -0.8013142818653432E+00 {~~}
688 START P 41 0.27382847600000001E+01 {~~}
689 START H burner 41 -0.2787914489945458E+03 {~~}
690 START Q burner 316 0.0000000000000000E+00 {~~}
691 START ZA burner 1 0.3585000230706632E+02 {~~}
692 START Y_J FLUE_GAS O2 0.1526526181100374E+00 {~~}
693 START Y_J FLUE_GAS N2 0.7311610583748572E+00 {~~}
694 START Y_J FLUE_GAS NO 0.0000000000000000E+00 {~~}
695 START Y_J FLUE_GAS CO2 0.4278561806047913E-01 {~~}
696 START Y_J FLUE_GAS H2O-G 0.6518498470280273E-01 {~~}
697 START Y_J FLUE_GAS SO2 0.0000000000000000E+00 {~~}
698 START Y_J FLUE_GAS NO2 0.0000000000000000E+00 {~~}
699 START Y_J FLUE_GAS AR 0.8215720751823488E-02 {~~}
700 START M GT 41 0.8013142818653432E+00 {~~}
701 START H GT 41 -0.2787914489945458E+03 {~~}
702 START M GT 42 -0.8013142818653432E+00 {~~}
703 START P 42 0.10380000000000000E+01 {~~}
704 START H GT 42 -0.5020368493447578E+03 {~~}
705 START W GT 117 -0.1788897276613712E+03 {~~}
706 START E generator 217 -0.6382224141371830E+02 {~~}
707 START Q generator 317 -0.3359065337564116E+01 {~~}
708 START W generator 117 0.6718130675128242E+02 {~~}
709 START M recuperator 42 0.8013142818653432E+00 {~~}
710 START H recuperator 42 -0.5020368493447578E+03 {~~}
711 START M recuperator 43 -0.8013142818653432E+00 {~~}
712 START H recuperator 43 -0.8735921928420305E+03 {~~}
713 START M recuperator 32 0.7181094385080242E+00 {~~}
714 START H recuperator 32 0.3066441581850383E+02 {~~}
715 START M recuperator 33 -0.7181094385080242E+00 {~~}
716 START H recuperator 33 0.4452705848535890E+03 {~~}
717 START Q recuperator 318 0.0000000000000000E+00 {~~}
718 START ZA recuperator 1 0.2977326032477479E+03 {~~}
719 START M exhaustcooler 430 0.8013142818653432E+00 {~~}
720 START H exhaustcooler 430 -0.9221860411687504E+03 {~~}
721 START M exhaustcooler 44 -0.8013142818653432E+00 {~~}
722 START P 44 0.10130000000000000E+01 {~~}
723 START H exhaustcooler 44 -0.1066378943833518E+04 {~~}
724 START M exhaustcooler 85 0.5524250302864077E+00 {~~}
725 START P 85 0.10130000000000000E+01 {~~}
726 START H exhaustcooler 85 -0.1584524528596511E+05 {~~}
727 START M exhaustcooler 86 -0.5524250302864077E+00 {~~}
728 START P 86 0.10080000000000000E+01 {~~}
729 START H exhaustcooler 86 -0.1563608779686837E+05 {~~}
730 START Q exhaustcooler 319 0.0000000000000000E+00 {~~}
731 START ZA exhaustcooler 1 0.1155438322488978E+03 {~~}
732 C ~~~~~
733 C ~~ End of generated initial guesses.
734 C ~~~~~
end

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DNA Output for optimized SOFC-MGT scenario

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1	Optimized Biomass gasification (Viking) + SOFC/MGT incl. recuperation												
2	RUN NUMBER 1												
3													
4													
5													
6	ALGEBRAIC VARIABLES												
7	NO	TO	MEDIA	M	T	P	H	ENERGY	X	S	V	U	
8	DE	COMPONENT		[kg/s]	[C]	[bar]	[kJ/kg]	[kJ/s]		[kJ/kg K]	[m3/kg]	[kJ/kg]	
9	-----												
10	1	Dryer	Wood	0.04	15.00	-	-8621.6	4.991E+02	-	0.4612	-	-8621.6	
11	64	Dryer	STEAM-HF	0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2	
12	2	Dryer	DryWood	-0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1	
13	61	Dryer	STEAM-HF	-0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1	
14	301	Dryer	HEAT					0.000E+00					
15	2	Gasifier	DryWood	0.03	150.00	-	-5497.1		-	1.7075	-	-5497.1	
16	26	Gasifier	STEAM-HF	0.00	150.00	1.003	-13194.5		-	11.1292	1.9309	-13388.2	
17	74	Gasifier	humid_air	0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7	
18	3	Gasifier	raw_PG	-0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1	
19	99	Gasifier	Ash	0.00	800.00	-	-4308.0		-	0.0000	-	-4308.0	
20	302	Gasifier	HEAT					0.000E+00					
21	3	airpreheat	raw_PG	0.09	800.00	0.998	-3507.9		-	10.8590	4.1308	-3920.1	
22	4	airpreheat	raw_PG	-0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7	
23	72	airpreheat	STANDARD_AIR	0.04	15.00	1.008	-98.8		-	6.8668	0.8237	-181.9	
24	73	airpreheat	STANDARD_AIR	-0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1	
25	303	airpreheat	HEAT					0.000E+00					
26	43	steamheater	FLUE_GAS	0.80	271.83	1.028	-873.6		-	7.6298	1.5330	-1031.2	
27	430	steamheater	FLUE_GAS	-0.80	226.65	1.023	-922.2		-	7.5381	1.4127	-1066.7	
28	63	steamheater	STEAM-HF	0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
29	64	steamheater	STEAM-HF	-0.20	250.00	0.998	-12996.5		-	11.5514	2.4110	-13237.2	
30	304	steamheater	HEAT					0.000E+00					
31	61	steamblower	STEAM-HF	0.21	150.00	0.993	-13194.4		-	11.1339	1.9505	-13388.1	
32	62	steamblower	STEAM-HF	-0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
33	305	steamblower	HEAT					-1.409E-02					
34	105	steamblower	MECH_POWER					7.044E-01					
35	62	split1	STEAM-HF	0.21	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
36	63	split1	STEAM-HF	-0.20	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
37	69	split1	STEAM-HF	-0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
38	73	mix1	STANDARD_AIR	0.04	780.00	1.003	724.5		-	8.2418	3.0255	421.1	
39	69	mix1	STEAM-HF	0.01	151.68	1.003	-13191.2		-	11.1370	1.9388	-13385.6	
40	74	mix1	humid_air	-0.05	564.13	1.003	-2398.8		-	9.1937	2.7302	-2672.7	
41	5	gascooler	raw_PG	0.09	256.76	0.988	-4379.3		-	9.7391	2.0604	-4582.9	
42	6	gascooler	cold_PG	-0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1	
43	98	gascooler	STEAM-HF	0.00	90.00	0.983	-15594.1		-	4.7085	0.0010	-15594.2	
44	81	gascooler	STEAM-HF	0.10	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3	
45	82	gascooler	STEAM-HF	-0.10	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2	
46	306	gascooler	HEAT					0.000E+00					
47	6	gasclean	cold_PG	0.09	90.00	0.983	-4624.6		-	9.1860	1.4192	-4764.1	
48	7	gasclean	clean_PG	-0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4	
49	97	gasclean	impurities	0.00	90.00	0.978	-535.6		-	6.2438	0.9059	-624.2	
50	307	gasclean	HEAT					0.000E+00					
51	7	condenser	clean_PG	0.09	90.00	0.978	-4624.9		-	9.1879	1.4263	-4764.4	
52	8	condenser	dry_PG	-0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1	
53	96	condenser	STEAM-HF	0.00	50.01	0.973	-15761.7		-	4.2198	0.0010	-15761.7	
54	83	condenser	STEAM-HF	0.05	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3	

DNA Output for optimized SOFC-MGT scenario

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55	84	condenser	STEAM-HF		-0.05	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
56	308	condenser	HEAT					0.000E+00					
57	8	PGcompressor	dry_PG		0.08	50.00	0.973	-4466.6		-	8.9598	1.2694	-4590.1
58	9	PGcompressor	dry_PG		-0.08	187.57	2.760	-4268.5		-	9.0714	0.6381	-4444.6
59	309	PGcompressor	HEAT					-3.363E-01					
60	117	PGcompressor	MECH_POWER					1.682E+01					
61	4	PGpreheat0	raw_PG		0.09	552.33	0.993	-3918.6		-	10.4262	3.1935	-4235.7
62	5	PGpreheat0	raw_PG		-0.09	256.76	0.988	-4379.3		-	9.7391	2.0604	-4582.9
63	9	PGpreheat0	dry_PG		0.08	187.57	2.760	-4268.5		-	9.0714	0.6381	-4444.6
64	90	PGpreheat0	dry_PG		-0.08	497.61	2.755	-3796.3		-	9.8532	1.0694	-4090.9
65	320	PGpreheat0	HEAT					0.000E+00					
66	11	PGpreheat	USEDFUEL		0.11	800.00	2.745	-6150.8		-	8.7788	1.1667	-6471.0
67	12	PGpreheat	USEDFUEL		-0.11	674.84	2.740	-6338.9		-	8.5930	1.0325	-6621.8
68	90	PGpreheat	dry_PG		0.08	497.61	2.755	-3796.3		-	9.8532	1.0694	-4090.9
69	10	PGpreheat	dry_PG		-0.08	650.00	2.750	-3551.2		-	10.1440	1.2832	-3904.1
70	311	PGpreheat	HEAT					0.000E+00					
71	31	aircompressor	STANDARD_AIR		0.72	15.00	1.013	-98.8		-	6.8653	0.8196	-181.9
72	32	aircompressor	STANDARD_AIR		-0.72	142.70	2.780	30.7		-	6.9463	0.4310	-89.2
73	312	aircompressor	HEAT					-1.898E+00					
74	117	aircompressor	MECH_POWER					9.489E+01					
75	42	recuperator	FLUE_GAS		0.80	602.36	1.038	-502.0		-	8.1583	2.4389	-755.2
76	43	recuperator	FLUE_GAS		-0.80	271.83	1.028	-873.6		-	7.6298	1.5330	-1031.2
77	32	recuperator	STANDARD_AIR		0.72	142.70	2.780	30.7		-	6.9463	0.4310	-89.2
78	33	recuperator	STANDARD_AIR		-0.72	533.41	2.770	445.3		-	7.6472	0.8390	212.9
79	318	recuperator	HEAT					0.000E+00					
80	35	airpreheat2	USEDAIR		0.69	800.00	2.750	746.2		-	7.9773	1.1285	435.9
81	36	airpreheat2	USEDAIR		-0.69	733.60	2.740	669.4		-	7.9045	1.0625	378.3
82	33	airpreheat2	STANDARD_AIR		0.72	533.41	2.770	445.3		-	7.6472	0.8390	212.9
83	34	airpreheat2	STANDARD_AIR		-0.72	600.00	2.760	519.4		-	7.7366	0.9116	267.8
84	314	airpreheat2	HEAT					0.000E+00					
85	10	sofc	dry_PG		0.08	650.00	2.750	-3551.2		-	10.1440	1.2832	-3904.1
86	34	sofc	STANDARD_AIR		0.72	600.00	2.760	519.4		-	7.7366	0.9116	267.8
87	11	sofc	USEDFUEL		-0.11	800.00	2.745	-6150.8		-	8.7788	1.1667	-6471.0
88	35	sofc	USEDAIR		-0.69	800.00	2.750	746.2		-	7.9773	1.1285	435.9
89	215	sofc	ELECT_POWER					-2.273E+02					
90	315	sofc	HEAT					0.000E+00					
91	36	burner	USEDAIR		0.69	733.60	2.740	669.4		-	7.9045	1.0625	378.3
92	12	burner	USEDFUEL		0.11	674.84	2.740	-6338.9		-	8.5930	1.0325	-6621.8
93	41	burner	FLUE_GAS		-0.80	790.13	2.738	-278.8		-	8.1087	1.1228	-586.2
94	316	burner	HEAT					0.000E+00					
95	41	GT	FLUE_GAS		0.80	790.13	2.738	-278.8		-	8.1087	1.1228	-586.2
96	42	GT	FLUE_GAS		-0.80	602.36	1.038	-502.0		-	8.1583	2.4389	-755.2
97	117	GT	MECH_POWER					-1.789E+02					
98	217	generator	ELECT_POWER					-6.382E+01					
99	317	generator	HEAT					-3.359E+00					
100	117	generator	MECH_POWER					6.718E+01					
101	430	exhaustcooler	FLUE_GAS		0.80	226.65	1.023	-922.2		-	7.5381	1.4127	-1066.7
102	44	exhaustcooler	FLUE_GAS		-0.80	90.02	1.013	-1066.4		-	7.2042	1.0367	-1171.4
103	85	exhaustcooler	STEAM-HF		0.55	30.02	1.013	-15845.2		-	3.9530	0.0010	-15845.3
104	86	exhaustcooler	STEAM-HF		-0.55	80.00	1.008	-15636.1		-	4.5912	0.0010	-15636.2
105	319	exhaustcooler	HEAT					0.000E+00					

DNA Output for optimized SOFC-MGT scenario

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108										
109	EXERGY									
110										
111	NO	TO	MEDIA	E_PH	E_CH	E	EX_PH	EX_CH	EX	
112	DE	COMPONENT		[kJ/kg]	[kJ/kg]	[kJ/kg]	[kJ/s]	[kJ/s]	[kJ/s]	
113	-----									
114	1	Dryer	Wood	0.00	13311.33	13311.33	0.00	572.39	572.39	
115	64	Dryer	STEAM-HF	660.71	-	660.71	132.17	-	132.17	
116	2	Dryer	DryWood	-54.56	18651.57	18597.01	1.67	-572.39	-570.71	
117	61	Dryer	STEAM-HF	583.11	-	583.11	-123.83	-	-123.83	
118	301	Dryer	HEAT	-	-	-	0.00	0.00	0.00	
119	2	Gasifier	DryWood	-54.56	18651.57	18597.01	-1.67	572.39	570.71	
120	26	Gasifier	STEAM-HF	584.41	-	584.41	0.00	-	0.00	
121	74	Gasifier	humid_air	310.33	66.40	376.73	17.02	3.64	20.66	
122	3	Gasifier	raw_PG	644.70	5438.32	6083.02	-54.98	-463.75	-518.73	
123	99	Gasifier	Ash	785.00	-	785.00	-0.21	-	-0.21	
124	302	Gasifier	HEAT	-	-	-	0.00	0.00	0.00	
125	3	airpreheat	raw_PG	644.70	5438.32	6083.02	54.98	463.75	518.73	
126	4	airpreheat	raw_PG	358.65	5438.32	5796.96	-30.58	-463.75	-494.34	
127	72	airpreheat	STANDARD_AIR	0.66	3.73	4.39	0.03	0.16	0.19	
128	73	airpreheat	STANDARD_AIR	427.84	3.73	431.57	-18.20	-0.16	-18.36	
129	303	airpreheat	HEAT	-	-	-	0.00	0.00	0.00	
130	43	steamheater	FLUE_GAS	79.89	21.69	101.58	64.02	17.38	81.40	
131	430	steamheater	FLUE_GAS	57.71	21.69	79.40	-46.25	-17.38	-63.62	
132	63	steamheater	STEAM-HF	585.47	-	585.47	117.12	-	117.12	
133	64	steamheater	STEAM-HF	660.71	-	660.71	-132.17	-	-132.17	
134	304	steamheater	HEAT	-	-	-	0.00	0.00	0.00	
135	61	steamblower	STEAM-HF	583.11	-	583.11	123.83	-	123.83	
136	62	steamblower	STEAM-HF	585.47	-	585.47	-124.33	-	-124.33	
137	305	steamblower	HEAT	-	-	-	0.00	0.00	0.00	
138	105	steamblower	MECH_POWER	-	-	-	0.70	0.00	0.70	
139	62	split1	STEAM-HF	585.47	-	585.47	124.33	-	124.33	
140	63	split1	STEAM-HF	585.47	-	585.47	-117.12	-	-117.12	
141	69	split1	STEAM-HF	585.47	-	585.47	-7.21	-	-7.21	
142	73	mix1	STANDARD_AIR	427.84	3.73	431.57	18.20	0.16	18.36	
143	69	mix1	STEAM-HF	585.47	-	585.47	7.21	-	7.21	
144	74	mix1	humid_air	310.33	66.40	376.73	-17.02	-3.64	-20.66	
145	5	gascooler	raw_PG	95.93	5438.32	5534.25	8.18	463.75	471.93	
146	6	gascooler	cold_PG	10.04	5438.32	5448.36	-0.86	-463.75	-464.61	
147	98	gascooler	STEAM-HF	34.93	-	34.93	0.00	-	0.00	
148	81	gascooler	STEAM-HF	1.49	-	1.49	0.15	-	0.15	
149	82	gascooler	STEAM-HF	26.73	-	26.73	-2.67	-	-2.67	
150	306	gascooler	HEAT	-	-	-	0.00	0.00	0.00	
151	6	gasclean	cold_PG	10.04	5438.32	5448.36	0.86	463.75	464.61	
152	7	gasclean	clean_PG	9.49	5437.03	5446.52	-0.81	-463.61	-464.42	
153	97	gasclean	impurities	6.93	23829.09	23836.02	0.00	-0.15	-0.15	
154	307	gasclean	HEAT	-	-	-	0.00	0.00	0.00	
155	7	condenser	clean_PG	9.49	5437.03	5446.52	0.81	463.61	464.42	
156	8	condenser	dry_PG	-0.23	5566.16	5565.93	0.02	-463.13	-463.11	
157	96	condenser	STEAM-HF	8.19	-	8.19	-0.02	-	-0.02	
158	83	condenser	STEAM-HF	1.49	-	1.49	0.07	-	0.07	
159	84	condenser	STEAM-HF	26.73	-	26.73	-1.25	-	-1.25	
160	308	condenser	HEAT	-	-	-	0.00	0.00	0.00	
161	8	PGcompressor	dry_PG	-0.23	5566.16	5565.93	-0.02	463.13	463.11	

DNA Output for optimized SOFC–MGT scenario

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161									
162	9	PGcompressor	dry_PG	165.67	5566.16	5731.83	-13.78	-463.13	-476.92
163	309	PGcompressor	HEAT	-	-	-	0.00	0.00	0.00
164	117	PGcompressor	MECH_POWER	-	-	-	16.82	0.00	16.82
165	4	PGpreheat0	raw_PG	358.65	5438.32	5796.96	30.58	463.75	494.34
166	5	PGpreheat0	raw_PG	95.93	5438.32	5534.25	-8.18	-463.75	-471.93
167	9	PGpreheat0	dry_PG	165.67	5566.16	5731.83	13.78	463.13	476.92
168	90	PGpreheat0	dry_PG	412.56	5566.16	5978.72	-34.33	-463.13	-497.46
169	320	PGpreheat0	HEAT	-	-	-	0.00	0.00	0.00
170	11	PGpreheat	USED_FUEL	655.16	787.09	1442.25	71.03	85.33	156.36
171	12	PGpreheat	USED_FUEL	520.57	787.09	1307.66	-56.44	-85.33	-141.77
172	90	PGpreheat	dry_PG	412.56	5566.16	5978.72	34.33	463.13	497.46
173	10	PGpreheat	dry_PG	573.90	5566.16	6140.06	-47.75	-463.13	-510.88
174	311	PGpreheat	HEAT	-	-	-	0.00	0.00	0.00
175	31	aircompressor	STANDARD_AIR	1.07	3.73	4.81	0.77	2.68	3.45
176	32	aircompressor	STANDARD_AIR	107.24	3.73	110.97	-77.01	-2.68	-79.69
177	312	aircompressor	HEAT	-	-	-	0.00	0.00	0.00
178	117	aircompressor	MECH_POWER	-	-	-	94.89	0.00	94.89
179	42	recuperator	FLUE_GAS	299.17	21.69	320.85	239.73	17.38	257.11
180	43	recuperator	FLUE_GAS	79.89	21.69	101.58	-64.02	-17.38	-81.40
181	32	recuperator	STANDARD_AIR	107.24	3.73	110.97	77.01	2.68	79.69
182	33	recuperator	STANDARD_AIR	319.88	3.73	323.61	-229.71	-2.68	-232.39
183	318	recuperator	HEAT	-	-	-	0.00	0.00	0.00
184	35	airpreheat2	USED_AIR	529.64	3.79	533.43	366.99	2.63	369.61
185	36	airpreheat2	USED_AIR	473.80	3.79	477.59	-328.29	-2.63	-330.92
186	33	airpreheat2	STANDARD_AIR	319.88	3.73	323.61	229.71	2.68	232.39
187	34	airpreheat2	STANDARD_AIR	368.27	3.73	372.00	-264.46	-2.68	-267.14
188	314	airpreheat2	HEAT	-	-	-	0.00	0.00	0.00
189	10	sofc	dry_PG	573.90	5566.16	6140.06	47.75	463.13	510.88
190	34	sofc	STANDARD_AIR	368.27	3.73	372.00	264.46	2.68	267.14
191	11	sofc	USED_FUEL	655.16	787.09	1442.25	-71.03	-85.33	-156.36
192	35	sofc	USED_AIR	529.64	3.79	533.43	-366.99	-2.63	-369.61
193	215	sofc	ELECT_POWER	-	-	-	-227.28	0.00	-227.28
194	315	sofc	HEAT	-	-	-	0.00	0.00	0.00
195	36	burner	USED_AIR	473.80	3.79	477.59	328.29	2.63	330.92
196	12	burner	USED_FUEL	520.57	787.09	1307.66	56.44	85.33	141.77
197	41	burner	FLUE_GAS	536.71	21.69	558.40	-430.07	-17.38	-447.45
198	316	burner	HEAT	-	-	-	0.00	0.00	0.00
199	41	GT	FLUE_GAS	536.71	21.69	558.40	430.07	17.38	447.45
200	42	GT	FLUE_GAS	299.17	21.69	320.85	-239.73	-17.38	-257.11
201	117	GT	MECH_POWER	-	-	-	-178.89	0.00	-178.89
202	217	generator	ELECT_POWER	-	-	-	-63.82	0.00	-63.82
203	317	generator	HEAT	-	-	-	0.00	0.00	0.00
204	117	generator	MECH_POWER	-	-	-	67.18	0.00	67.18
205	430	exhaustcooler	FLUE_GAS	57.71	21.69	79.40	46.25	17.38	63.62
206	44	exhaustcooler	FLUE_GAS	9.74	21.69	31.43	-7.81	-17.38	-25.19
207	85	exhaustcooler	STEAM-HF	1.49	-	1.49	0.83	-	0.83
208	86	exhaustcooler	STEAM-HF	26.73	-	26.73	-14.77	-	-14.77
209	319	exhaustcooler	HEAT	-	-	-	0.00	0.00	0.00
210	-----								
211									
212	ELEC. POWER PRODUCTION =			291.1022 kW					
213	TOTAL POWER CONSUMPTION =			0.7044 kW					
214	NET POWER PRODUCTION =			290.3978 kW					

DNA Output for optimized SOFC–MGT scenario

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215 FUEL CONSUMPTION (LHV) = 499.1161 kJ/s
216 FUEL CONSUMPTION (HHV) = 572.3872 kJ/s
217 THERMAL EFFICIENCY (LHV)= 0.5818
218 THERMAL EFFICIENCY (HHV)= 0.5073
219
220 MAXIMUM RELATIVE ERROR = 9.0091E-13
221 COMPUTER ACCURACY = 1.0842E-19
222
223
224
225 IDEAL GAS COMPOSITION (MOLAR BASE):
226
227 |humid_air |raw_PG |STANDARD_AIR|FLUE_GAS |cold_PG |
228 -----
229 HYDROGEN | 0.0000E+00 | 0.2538E+00 | 0.0000E+00 | 0.0000E+00 | 0.2538E+00 |
230 OXYGEN | 0.1418E+00 | 0.0000E+00 | 0.2075E+00 | 0.1527E+00 | 0.0000E+00 |
231 NITROGEN | 0.5281E+00 | 0.2897E+00 | 0.7729E+00 | 0.7312E+00 | 0.2897E+00 |
232 CARBON MONOXIDE | 0.0000E+00 | 0.1762E+00 | 0.0000E+00 | 0.0000E+00 | 0.1762E+00 |
233 CARBON DIOXIDE | 0.2050E-03 | 0.1144E+00 | 0.3000E-03 | 0.4279E-01 | 0.1144E+00 |
234 WATER (I.G.) | 0.3236E+00 | 0.1523E+00 | 0.1010E-01 | 0.6518E-01 | 0.1523E+00 |
235 HYDROGEN SULFIDE| 0.0000E+00 | 0.4616E-04 | 0.0000E+00 | 0.0000E+00 | 0.4616E-04 |
236 METHANE | 0.0000E+00 | 0.1011E-01 | 0.0000E+00 | 0.0000E+00 | 0.1011E-01 |
237 ARGON | 0.6286E-02 | 0.3444E-02 | 0.9200E-02 | 0.8216E-02 | 0.3444E-02 |
238 -----
239 MEAN MOLE MASS| 0.2542E+02 | 0.2164E+02 | 0.2885E+02 | 0.2875E+02 | 0.2164E+02 |
240 NET CALORI VALUE| 0.0000E+00 | 0.5516E+04 | 0.0000E+00 | 0.0000E+00 | 0.5516E+04 |
241 GRS CALORI VALUE| 0.0000E+00 | 0.1148E+05 | 0.0000E+00 | 0.0000E+00 | 0.1148E+05 |
242 -----
243
244 IDEAL GAS COMPOSITION (MOLAR BASE):
245
246 |clean_PG |impurities |dry_PG |USED_FUEL |USED_AIR |
247 -----
248 HYDROGEN | 0.2538E+00 | 0.0000E+00 | 0.2614E+00 | 0.3681E-01 | 0.0000E+00 |
249 OXYGEN | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.1816E+00 |
250 NITROGEN | 0.2897E+00 | 0.0000E+00 | 0.2983E+00 | 0.2933E+00 | 0.7982E+00 |
251 CARBON MONOXIDE | 0.1762E+00 | 0.0000E+00 | 0.1815E+00 | 0.2593E-01 | 0.0000E+00 |
252 CARBON DIOXIDE | 0.1144E+00 | 0.0000E+00 | 0.1179E+00 | 0.2786E+00 | 0.3098E-03 |
253 WATER (I.G.) | 0.1523E+00 | 0.0000E+00 | 0.1269E+00 | 0.3654E+00 | 0.1043E-01 |
254 HYDROGEN SULFIDE| 0.0000E+00 | 0.1000E+01 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
255 METHANE | 0.1011E-01 | 0.0000E+00 | 0.1042E-01 | 0.1599E-06 | 0.0000E+00 |
256 ARGON | 0.3444E-02 | 0.0000E+00 | 0.3547E-02 | 0.0000E+00 | 0.9501E-02 |
257 -----
258 MEAN MOLE MASS| 0.2164E+02 | 0.3408E+02 | 0.2175E+02 | 0.2786E+02 | 0.2875E+02 |
259 NET CALORI VALUE| 0.5515E+04 | 0.1521E+05 | 0.5652E+04 | 0.5829E+03 | 0.0000E+00 |
260 GRS CALORI VALUE| 0.1148E+05 | 0.1650E+05 | 0.1172E+05 | 0.2279E+04 | 0.0000E+00 |
261 -----
262
263 NON-IDEAL FLUID AND SOLID COMPOSITION (MASS BASE):
264
265 |Wood |DryWood |Ash |
266 -----
267 HYDROGEN | 0.4204E-01 | 0.5890E-01 | 0.0000E+00 |
268 OXYGEN | 0.2976E+00 | 0.4171E+00 | 0.0000E+00 |
```

DNA Output for optimized SOFC–MGT scenario

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```
268
269 NITROGEN      | 0.1153E-02 | 0.1615E-02 | 0.0000E+00 |
270 CARBON (SOLID) | 0.3309E+00 | 0.4636E+00 | 0.0000E+00 |
271 SULFUR (SOLID) | 0.1356E-03 | 0.1900E-03 | 0.0000E+00 |
272 WATER (LIQUID) | 0.3220E+00 | 0.5000E-01 | 0.0000E+00 |
273 ASHES         | 0.6170E-02 | 0.8645E-02 | 0.1000E+01 |
274 -----
275 MEAN MOLE MASS| 0.1321E+02 | 0.1193E+02 | 0.7600E+02 |
276 NET CALORI VALUE| 0.1161E+05 | 0.1724E+05 | 0.0000E+00 |
277 GRS CALORI VALUE| 0.1331E+05 | 0.1865E+05 | 0.0000E+00 |
278 -----
279
280 MEDIUM 97 : WATER FOR GAS APP
281 MEDIUM 300 : HEAT
282 MEDIUM 301 : PRODUCT HEAT
283
284
285 NUMBER OF CLOSED INTERNAL LOOPS IN THE SYSTEM: 0
286
287
288
289
290
291 SOLUTION FOR THE INDEPENDENT ALGEBRAIC VARIABLES :
292
293
294 VARIABLE NO | COMPONENT | NAME | VALUE |
295 -----
296 1 |Gasifier |MULTIPLIER H| 0.8501E+05 |
297 2 |Gasifier |MULTIPLIER C| 0.4364E+05 |
298 3 |Gasifier |MULTIPLIER N| 0.1173E+06 |
299 4 |Gasifier |MULTIPLIER O| 0.3125E+06 |
300 5 |Gasifier |MULTIPLIER S| 0.1828E+06 |
301 6 |Gasifier |MULTIPL Ar | 0.2292E+06 |
302 7 |Gasifier |GIBBS ENERGY| -.3280E+06 |
303 1 |airpreheat |Transferred | 0.3503E+02 |
304 1 |steamheater |Transferred | 0.3894E+02 |
305 1 |PGpreheat0 |Transferred | 0.3929E+02 |
306 1 |PGpreheat |Transferred | 0.2039E+02 |
307 1 |recuperator |Transferred | 0.2977E+03 |
308 1 |airpreheat2 |Transferred | 0.5324E+02 |
309 1 |sofc |MULTIPLIER H| 0.8911E+05 |
310 2 |sofc |MULTIPLIER C| 0.7674E+05 |
311 3 |sofc |MULTIPLIER N| 0.1127E+06 |
312 4 |sofc |MULTIPLIER O| 0.2875E+06 |
313 5 |sofc |GIBBS ENERGY| -.4338E+06 |
314 6 |sofc |ETAMAX | 0.7046E+00 |
315 7 |sofc |ETASYS | 0.8494E+00 |
316 8 |sofc |UF | 0.8500E+00 |
317 9 |sofc |ETATOT | 0.5087E+00 |
318 10 |sofc |STCR | 0.4098E+00 |
319 11 |sofc |E_nernst | 0.9675E+00 |
320 12 |sofc |V_act | 0.1081E+00 |
321 13 |sofc |V_ohm | 0.7147E-02 |
322 14 |sofc |V_conc | 0.3043E-01 |
```

DNA Output for optimized SOFC–MGT scenario

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```
322
323      15      |sofc      |V_cell      | 0.8218E+00 |
324      16      |sofc      |GMAX        | -.8662E+05 |
325      17      |sofc      |G(T)        | -.1885E+06 |
326      18      |sofc      |G(p,T)      | -.1867E+06 |
327      19      |sofc      |p_H2eq      | 0.7518E+00 |
328      20      |sofc      |R_e         | 0.2336E-01 |
329      21      |sofc      |Area [cm^2] | 0.1013E+04 |
330      22      |sofc      |i_load      | 0.3000E+03 |
331      23      |sofc      |eta_DCAC    | 0.9500E+00 |
332      1       |burner     |Lambda      | 0.3585E+02 |
333      1       |exhaustcooler |Transferred | 0.1155E+03 |
334 -----
335
336 =====
337 #####
end
```

Appendix G PAPER I

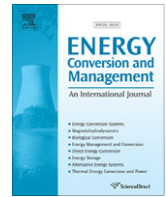
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Thermodynamic performance study of biomass gasification, solid oxide fuel cell and micro gas turbine hybrid systems

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ABSTRACT

A system level modelling study of three combined heat and power systems based on biomass gasification is presented. Product gas is converted in a micro gas turbine (MGT) in the first system, in a solid oxide fuel cell (SOFC) in the second system and in a combined SOFC–MGT arrangement in the third system. An electrochemical model of the SOFC has been developed and calibrated against published data from Topsoe Fuel Cells A/S and the Risø National Laboratory. The modelled gasifier is based on an up scaled version ($\sim 500 \text{ kW}_{\text{th}}$) of the demonstrated low tar gasifier, Viking, situated at the Technical University of Denmark. The SOFC converts the syngas more efficiently than the MGT, which is reflected by the energetic electrical efficiency of the gasifier and MGT system in opposition to the gasifier and SOFC configuration – $\eta_{\text{el}} = 28.1\%$ versus $\eta_{\text{el}} = 36.4\%$. By combining the SOFC and MGT, the unconverted syngas from the SOFC is utilised in the MGT to produce more power and the SOFC is pressurised, which improves the efficiency to as much as $\eta_{\text{el}} = 50.3\%$. Variation of the different operating conditions reveals an optimum for the chosen pressure ratio with respect to the resulting electrical efficiency. Furthermore, the SOFC operating temperature should be kept high and the cathode temperature gradient maximised.

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1. Introduction

Development of sustainable and efficient production plants with combined heat and power (CHP) have gained more attention as climate change and the security of the supply and depletion of fossil fuels have become increasingly well-known issues. The share of biomass in CHP production is expected to increase in the future and decentralised CHP plants are of interest to avoid the cost associated with biomass transportation. Efficient power producing technologies for small scale production typically include gas engines, micro gas turbines (MGT) and fuel cells – all of which require gaseous fuel. Gasification can deliver biomass-based gaseous fuel. Therefore, combining biomass gasification and efficient syngas conversion may enable the design of a sustainable and efficient CHP plant.

Solid oxide fuel cells (SOFCs) can electrochemically convert H_2 and CO as well as internally reform CH_4 into more H_2 and CO due to their high operating temperature and the presence of a nickel catalyst. These conversions make SOFCs very fuel flexible and ideal for syngas conversion compared to other fuel cell types.

The performance and system design of integrated biomass gasifier and SOFC systems have been investigated by several researchers – first by Alderucci et al. in 1994 [1] and later by others [2–4].

An alternative design including heat pipes to thermally integrate an SOFC stack and an allothermal gasifier have also been published [5–8]. A major issue of combining gasification and SOFCs has proved to be gas cleaning, as SOFCs have strict requirements for fuel cleanliness [9,10].

Usage of gas turbine technology in combination with biomass gasification and SOFCs to improve system performance has also been shown. Efficiencies near 60% (LHV) should be achievable for large scale plants in the 5 MW_e class [11]. A few researchers have looked at small scale plants using MGTs [7,12,13], but Fryda et al. [13] was the only group to compare the performance of a hybrid CHP system consisting of an autothermal gasifier feeding either an MGT, an SOFC or both combined. The best performing coupling used both the SOFC and MGT and obtained an electrical efficiency of approximately 40% (LHV).

This study focus on the potential of using the concept of a demonstrated two stage autothermal (air blown) fixed bed biomass gasifier in a small scale CHP plant ($\sim 500 \text{ kW}_{\text{th}}$) together with an SOFC and/or MGT. This gasifier plant, named Viking, produces a very clean gas, avoiding the need for advanced gas cleaning, and performs with a high cold gas efficiency of 93%. Viking was developed at the Technical University of Denmark and is demonstrated in a size of 75 kW_{th} integrated with a gas engine performing with a biomass to electricity efficiency of approximately 25% (LHV). Details of this plant can be found in [14,15]. Hofmann et al. [16] operated an SOFC on cleaned syngas from the Viking gasifier for 150 h

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Nomenclature

a_{ohm}	coefficient ($\text{k}\Omega \text{ cm}$)
b_{ohm}	coefficient (K)
CC	carbon conversion factor (–)
E_{act}	activation energy (J mol^{-1})
E	reversible open circuit voltage (V)
ex	exergy (W)
F	Faradays constant (C mol^{-1})
g_f	Gibbs free energy (J mol^{-1})
h_f	enthalpy of formation (J mol^{-1})
i	current density (mA cm^{-2})
i_n	internal current density (mA cm^{-2})
i_0	exchange current density (mA cm^{-2})
LHV	lower heating value (kJ kg^{-1})
\dot{m}	mass flow (kg s^{-1})
METH	fraction of non-equilibrium methane (–)
\dot{n}	molar flow (mol s^{-1})
n_e	number of transferred electrons for each molecule of fuel (–)
p	pressure (bar)
P	power production (W)
PR	pressure ratio (–)
Q_{DH}	district heating production (J s^{-1})
r	area specific resistance of one or all layers ($\text{k}\Omega \text{ cm}^2$)
R	universal gas constant ($\text{J K}^{-1} \text{ mol}^{-1}$)
T	temperature (K)
U_F	fuel utilisation factor for fuel cell (%)
V	potential/overpotential (V)
x	mass fraction (–)
y	molar fraction (–)

Greek letters

δ	fuel cell layer thickness (cm)
Δ	change/difference
η_{CHP}	energy based combined heat and power efficiency (%)
η_{cg}	cold gas efficiency of gasifier (%)
η_{el}	energy based electrical efficiency (%)
$\eta_{\text{ex,CHP}}$	exergy based combined heat and power efficiency (%)
$\eta_{\text{ex,el}}$	exergy based electrical efficiency (%)
η_{rev}	reversible fuel cell efficiency (%)
η_v	voltage efficiency of fuel cell (%)
γ	exchange current density constant (mA cm^{-2})
ρ	resistivity ($\text{k}\Omega \text{ cm}$)

Superscript

0	standard conditions
---	---------------------

Subscripts

a	anode
act	activation
c	cathode
C	carbon
cell	single fuel cell
con	consumption
e	electrolyte
elec	electrode
i	interconnect
in	inlet stream
ohm	ohmic
out	outlet stream
th	thermal
tot	total

without degradation. Furthermore, the impacts of varying the operating conditions of the SOFC and MGT are studied and discussed and the sensitivity of the total electrical system efficiency to these operating conditions are examined. From an electrical efficiency point of view, the optimal operating conditions are clarified. Economic aspects will influence the feasibility of the studied plant concepts, but economics are without the scope of this work and, as SOFCs are not fully commercialised, the future cost of SOFCs is uncertain.

The present study is based on steady-state process modelling combining zero-dimensional component models using the simulation tool Dynamic Network Analysis (DNA) [17]. DNA, which was developed at The Technical University of Denmark, is a component-based tool that incorporates thermodynamic property data.

A component model of the SOFC has been developed for the purpose of this study. The SOFC model includes an electrochemical model and takes the operating conditions of the SOFC, e.g., the operating temperature and pressure as well as the gas composition, fuel utilisation and load (current density), into account when predicting the SOFC performance.

2. System description

Three combined heat and power system configurations are investigated in this study. They are based on syngas production from an up scaled Viking gasifier. A flow sheet of the three systems is depicted in Fig. 1. The modelled gasifier system is slightly simplified, but it aims at the same resulting gas composition and cold gas efficiency as the Viking gasifier. In the modelled gasifier, the dryer is heated by hot syngas. The steam production from the dryer is

added to the preheated air, and dry wood together with mixed air and steam are fed to the gasifier. The raw product gas is cooled to 90 °C in three steps, including air preheating, wood drying and syngas cooling, which produce hot water for district heating. The cooled syngas is then cleaned to remove impurities, such as particles, before some of the water in the gas is condensed through cooling to 50 °C. The cleaned and partly dried syngas is then converted into electricity and heat in a bottoming cycle consisting of an SOFC, an MGT or a combination of both the SOFC and the MGT. These three system configurations will be referred as the Gasifier–MGT, Gasifier–SOFC and Gasifier–SOFC–MGT configuration, respectively. In the Gasifier–SOFC–MGT configuration, all of the components in the flow sheet are in use, see Fig. 1. With respect to Fig. 1, the recuperator and gas turbine expander are bypassed in the Gasifier–SOFC case, whereas the SOFC and preheaters are bypassed in the Gasifier–MGT arrangement. Thus, the syngas and air compressors work as blowers in the Gasifier–SOFC case due to the lack of pressurisation. In addition, the syngas compressor works as a suction blower for the gasifier system. A generator (not illustrated) is situated on the axis of the gas turbine and it produces the net electric MGT power. In the Gasifier–SOFC configuration, the syngas and air blowers are driven by an electric motor.

3. Plant model

3.1. Gasifier model

The gasifier component calculates the produced syngas composition and produced ashes based on the inlet media composition and the operating conditions. The input parameters defining the

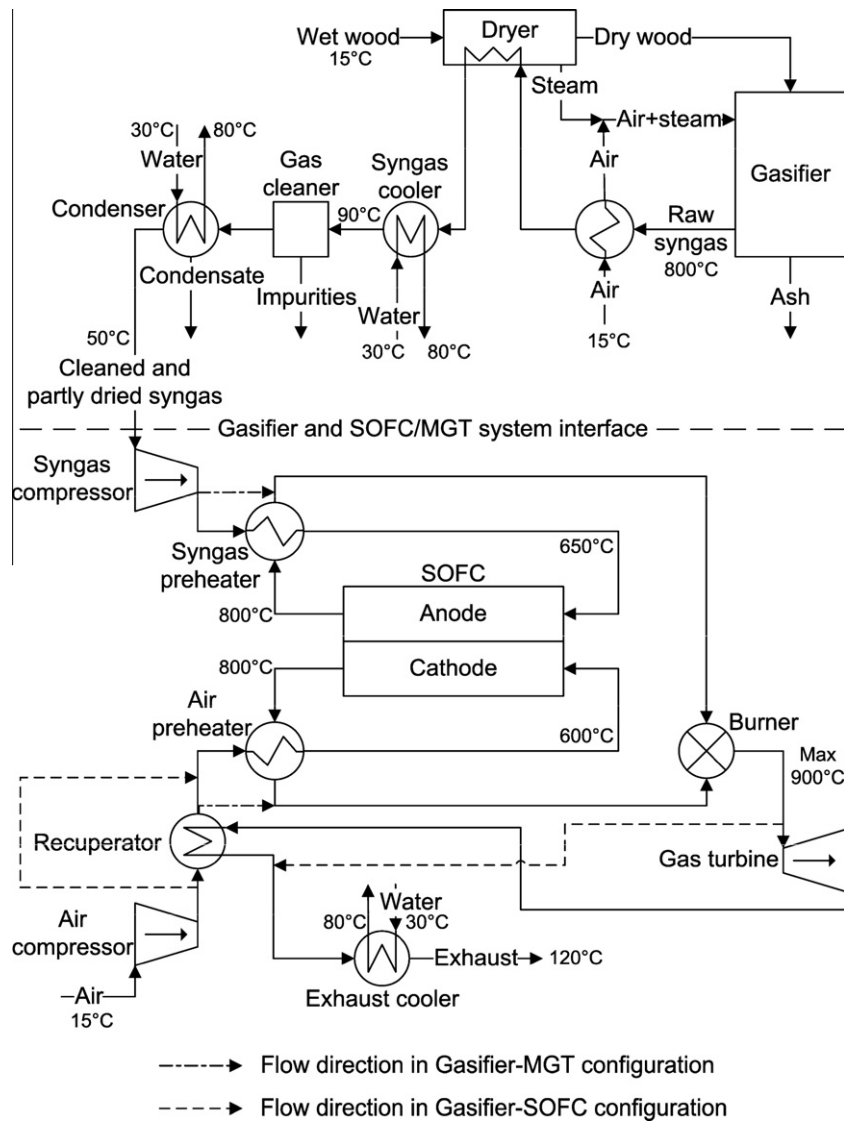


Fig. 1. Flow sheet of the gasifier system with SOFC and/or MGT.

Table 1
Inputs to the gasifier submodel.

Operating pressure	p_{gasifier}^a	0.998 bar
Operating temperature	T_{gasifier}^a	800 °C
Pressure loss	$\Delta p_{\text{gasifier}}$	5 mbar
Carbon conversion factor	CC	1
Non-equilibrium methane	METH	0.01

^a Equals the gasifier outlet.

operating conditions for the gasifier submodel are given in Table 1. The gasifier pressure loss is defined as the difference between the inlet air and steam mixture and the outlet syngas.

In the gasifier, the incoming flows are converted into syngas and ashes. The ashes are represented by SiO_2 and unconverted carbon. SiO_2 originates from a defined content in the inlet biomass, while the unconverted carbon is controlled by a defined carbon conversion factor (CC). The amount and composition of ash are calculated by the following equations:

$$\dot{m}_{\text{ash,out}} = \dot{m}_{\text{wood,in}} [x_{\text{SiO}_2,\text{in}} + x_{\text{C,in}} (1 - \text{CC})] \quad (1)$$

$$x_{\text{SiO}_2,\text{out}} = \frac{\dot{m}_{\text{wood,in}} x_{\text{SiO}_2,\text{in}}}{\dot{m}_{\text{ash,out}}} \quad (2)$$

$$x_{\text{C,out}} = 1 - x_{\text{SiO}_2,\text{out}} \quad (3)$$

The syngas can consist of the following species: H_2 , N_2 , CO , CO_2 , H_2O , CH_4 , H_2S and Ar. It is assumed that chemical equilibrium is reached at the operating temperature and pressure, where the total Gibbs free energy is minimised. With this assumption, the syngas outlet composition can be found by the Gibbs free energy minimisation method [18]. An option for bypassing methane in the equilibrium calculations is included in order to reach syngas compositions, which contain more methane than in the corresponding composition at equilibrium. Thus, the syngas composition can be adjusted to match realistic syngas compositions, e.g., from the Viking gasifier. The input parameter METH is used for this bypass option and is defined as the fraction of methane that is not included in the equilibrium calculations and instead appears in the outlet syngas.

3.1.1. Gasifier model validation

Model validation for the gasifier is done for the entire gasification plant, from the biomass input to the cleaned and dried syngas. Thus, data from the Viking gasifier plant can be used for validation.

Wood chips from beech with small amounts of oak are used in the model, which is in line with the wood chips used in the Viking gasifier reported in Ahrenfeldt et al. [15]. As seen in Table 2, the

Table 2

Dry syngas composition, LHV and cold gas efficiency for the Viking gasifier and the modelled gasifier.

	Viking gasifier [15]	Gasifier model
H ₂ (vol.%)	30.5	29.9
CO (vol.%)	19.6	20.8
CO ₂ (vol.%)	15.4	13.5
CH ₄ (vol.%)	1.16	1.19
N ₂ (vol.%)	33.3	34.2
LHV (MJ kg ⁻¹)	6.2	6.3
Cold gas efficiency (%)	93	94

produced syngas composition and the lower heating value (LHV) from the gasifier model are close to the Viking data. The CO₂ content shows the greatest variance, whereas the resulting LHVs are similar. The overall performance of the modelled gasifier is also similar to that of the Viking gasifier, as indicated by the cold gas efficiencies. The cold gas efficiency is defined in Eq. (4). The value of the cold gas efficiency is higher than traditional downdraft gasifiers, but it is ensured by the two stage design [15].

$$\eta_{\text{cold gas}} = \frac{\dot{m}_{\text{cold product gas}} \text{LHV}_{\text{cold product gas}}}{\dot{m}_{\text{biomass}} \text{LHV}_{\text{biomass}}} \quad (4)$$

3.2. Solid oxide fuel cell model

The SOFC stack component calculates the air and fuel outlet compositions and the power production. The calculations are based on the inlet air and fuel compositions and flow rates as well as the other operating conditions of the SOFC. The SOFC submodel includes an electrochemical model for predicting the performance of the SOFC. The operating conditions are partly described by input parameters given to the SOFC submodel. These parameters are presented in Table 3.

In the submodel only H₂ is electrochemically converted in the SOFC anode, but the model takes into account that CO produces an extra H₂ molecule through the water–gas–shift (WGS) reaction, while four additional H₂ molecules are produced from CH₄ through internal steam reforming and WGS of produced CO (full conversion is assumed). The total molar flow of H₂ on the anode after internal steam reforming and WGS is expressed in the following equation:

$$\dot{n}_{\text{H}_2, \text{tot}} = \dot{n}_{\text{H}_2, \text{in}} + \dot{n}_{\text{CO}, \text{in}} + 4\dot{n}_{\text{CH}_4, \text{in}} \quad (5)$$



The amount of H₂ that is electrochemically converted depends on the fuel utilisation factor (U_F). The electrode reactions and the overall fuel cell reaction are as shown in Eqs. (6)–(8).

The overall fuel cell reaction reveals that the amount of consumed O₂ is half the amount of consumed H₂. The cathode outlet composition is calculated by the following equations; the only species taken into account are O₂, N₂, CO₂, H₂O and Ar.

Table 3

Inputs to the SOFC submodel.

Fuel utilisation factor	U_F	0.85
Operating temperature	T_{SOFC}^a	800 °C
Anode pressure loss	Δp_a	5 mbar
Cathode pressure loss	Δp_c	10 mbar
Current density	i	300 mA cm ⁻²

^a Equals the SOFC anode and cathode outlets.

$$\dot{n}_{\text{O}_2, \text{con}} = \frac{U_F \dot{n}_{\text{H}_2, \text{in}}}{2} \quad (9)$$

$$\dot{n}_{\text{c}, \text{out}} = \dot{n}_{\text{c}, \text{in}} - \dot{n}_{\text{O}_2, \text{con}} \quad (10)$$

$$y_{\text{O}_2, \text{out}} = \frac{\dot{n}_{\text{c}, \text{in}} y_{\text{O}_2, \text{in}} - \dot{n}_{\text{O}_2, \text{con}}}{\dot{n}_{\text{c}, \text{out}}} \quad (11)$$

$$y_{j, \text{out}} = \frac{\dot{n}_{\text{c}, \text{in}} y_{j, \text{in}}}{\dot{n}_{\text{c}, \text{out}}}, \quad j = \{\text{N}_2, \text{CO}_2, \text{H}_2\text{O}\} \quad (12)$$

$$y_{\text{Ar}, \text{out}} = 1 - y_{\text{O}_2, \text{out}} - y_{\text{N}_2, \text{out}} - y_{\text{CO}_2, \text{out}} - y_{\text{H}_2\text{O}, \text{out}} \quad (13)$$

The fuel composition leaving the anode is calculated by the Gibbs free energy minimisation method [18] as described for the gasifier submodel. Chemical equilibrium at the anode outlet temperature and pressure is assumed for the following species: H₂, CO, CO₂, H₂O, CH₄ and N₂. The equilibrium assumption is fair because the methane content in this study is low.

Power production from the SOFC depends on the amount of chemical energy fed to the anode, the reversible efficiency (η_{rev}), the voltage efficiency (η_v) and the fuel utilisation factor (U_F). It is defined in mathematical form in the following equation:

$$P_{\text{SOFC}} = [(\Delta \bar{h}_f)_{\text{H}_2} \dot{n}_{\text{H}_2, \text{in}} + (\Delta \bar{h}_f)_{\text{CO}} \dot{n}_{\text{CO}, \text{in}} + (\Delta \bar{h}_f)_{\text{CH}_4} \dot{n}_{\text{CH}_4, \text{in}}] \eta_{\text{rev}} \eta_v U_F \quad (14)$$

The reversible efficiency is the maximum possible efficiency defined as the relationship between the maximum available electrical energy (change in Gibbs free energy) and the change in enthalpy of formation, both of which are associated with full oxidation of the fuel. This relationship is shown in the following equation:

$$\eta_{\text{rev}} = \frac{(\Delta \bar{g}_f)_{\text{fuel}}}{(\Delta \bar{h}_f)_{\text{fuel}}} \quad (15)$$

In this model, the change in enthalpy of formation is the LHV. The voltage efficiency expresses the electrochemical performance of the SOFC. The calculation of voltage efficiency is described in the following section.

3.2.1. Electrochemical model

The electrochemical model is used to calculate the cell potential and voltage efficiency of the SOFC. Both of these values depend on the operating conditions, including the temperature, pressure, gas compositions, fuel utilisation and load (current density). The cell potential and voltage efficiency are defined in Eqs. (16) and (17), respectively.

$$V_{\text{cell}} = E - V_{\text{act}} - V_{\text{ohm}} \quad (16)$$

$$\eta_v = \frac{V_{\text{cell}}}{E} \quad (17)$$

In the following part of the section, the reversible open circuit voltage (E), activation overpotential (V_{act}) and ohmic overpotential (V_{ohm}) are calculated. The concentration overpotential due to the limitation of gas diffusion between the gas channel and the active cell area is neglected in this study because operation at high current densities is not examined. The concentration overpotential does not normally contribute to excessive voltage loss unless the current density approaches the limiting current density [19].

E can be calculated from the Nernst equation:

$$E = \frac{-\Delta \bar{g}_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{\bar{p}_{\text{H}_2, \text{tot}} \sqrt{\bar{p}_{\text{O}_2}}}{\bar{p}_{\text{H}_2\text{O}}} \right) \quad (18)$$

Because it is assumed that all CO and CH₄ are converted to H₂ before the electrochemical reactions take place, the change in standard Gibbs free energy ($\Delta \bar{g}_f^0$) and the number of electrons transferred for each molecule of fuel (n_e) are determined for the reaction of H₂ only. Thus, $n_e = 2$ and $\Delta \bar{g}_f^0 = (\bar{g}_f^0)_{\text{H}_2\text{O}} - (\bar{g}_f^0)_{\text{H}_2} - 1/2(\bar{g}_f^0)_{\text{O}_2}$. The partial pressure of species j is an average

across the respective electrode and is defined as an arithmetic mean between the inlet and outlet shown in Eqs. (19) and (20). The average partial pressure of the available hydrogen after internal steam reforming and water gas shift of CH_4 and CO is defined in Eq. (21).

$$\bar{p}_j = \left(\frac{y_{j,\text{out}} - y_{j,\text{in}}}{2} \right) \bar{p}_a, \quad j = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2\} \quad (19)$$

$$\bar{p}_{\text{O}_2} = \left(\frac{y_{\text{O}_2,\text{out}} - y_{\text{O}_2,\text{in}}}{2} \right) \bar{p}_c \quad (20)$$

$$\bar{p}_{\text{H}_2,\text{tot}} = \bar{p}_{\text{H}_2} + \bar{p}_{\text{CO}} + 4\bar{p}_{\text{CH}_4} \quad (21)$$

The activation overpotential is due to an energy barrier (activation energy) that the reactants must overcome in order to drive the electrochemical reactions. The activation overpotential is non-linear and is dominant at low current densities (i). The activation overpotential is defined as (cf. [20]):

$$V_{\text{act}} = V_{\text{act},a} + V_{\text{act},c} = \frac{2RT}{n_e F} \left[\sinh^{-1} \left(\frac{i + i_n}{2i_{0,a}} \right) + \sinh^{-1} \left(\frac{i + i_n}{2i_{0,c}} \right) \right] \quad (22)$$

The internal current density (i_n) is added to the actual fuel cell current density in order to account for the mixed potential caused by fuel crossover. The importance of the internal current density in the case of SOFCs is much less than that for low temperature fuel cells. Moreover, the value of i_n is usually very small for SOFCs [21]. In this study, the value of i_n is 2 mA cm^{-2} [22]. The exchange current density (i_0) is a measure of the level of activity on the electrode at $i = 0 \text{ mA cm}^{-2}$ and is defined for the anode and cathode, respectively, as (cf. [23–25]):

$$i_{0,a} = \gamma_a \left(\frac{\bar{p}_{\text{H}_2,\text{tot}}}{\bar{p}_a} \right) \left(\frac{\bar{p}_{\text{H}_2\text{O}}}{\bar{p}_a} \right) \exp \left(\frac{-E_{\text{act},a}}{RT} \right) \quad (23)$$

$$i_{0,c} = \gamma_c \left(\frac{\bar{p}_{\text{O}_2}}{\bar{p}_c} \right)^{0.25} \exp \left(\frac{-E_{\text{act},c}}{RT} \right) \quad (24)$$

The values of γ and E_{act} can be found in Table 4.

The ohmic overpotential is caused by the electrical resistance towards the ions passing through the electrolyte and the electrons passing through the electrodes and interconnects. The ohmic overpotential is defined below.

$$V_{\text{ohm}} = i r_{\text{tot}} \quad (25)$$

$$r_{\text{tot}} = r_a + r_c + r_e + r_i \quad (26)$$

$$r_j = \delta_j \rho_j, \quad j = \{a, c, e, i\} \quad (27)$$

$$\rho_j = a_{\text{ohm},j} \exp \left(\frac{b_{\text{ohm},j}}{T} \right), \quad j = \{a, c, e, i\} \quad (28)$$

Table 4
Inputs for the electrochemical model.

R	$8.314 \text{ J K}^{-1} \text{ mol}^{-1}$	[22]
F	$96,485 \text{ C mol}^{-1}$	[22]
n_e	2	[22]
i_n	2 mA cm^{-2}	[22]
γ_a	$2.13 \times 10^7 \text{ mA cm}^{-2}$	[22]
γ_c	$1.49 \times 10^7 \text{ mA cm}^{-2}$	[22]
$E_{\text{act},a}$	$110,000 \text{ J mol}^{-1}$	[22]
$E_{\text{act},c}$	$110,000 \text{ J mol}^{-1}$	[22]
δ_a	$750 \times 10^{-4} \text{ cm}$	[19]
δ_c	$50 \times 10^{-4} \text{ cm}$	[19]
δ_e	$40 \times 10^{-4} \text{ cm}$	[19]
δ_i	$100 \times 10^{-4} \text{ cm}$	[26]
$a_{\text{ohm},a}$	$0.00298 \times 10^{-3} \text{ k}\Omega \text{ cm}$	[27]
$b_{\text{ohm},a}$	-1392 K	[27]
$a_{\text{ohm},c}$	$0.00811 \times 10^{-3} \text{ k}\Omega \text{ cm}$	[27]
$b_{\text{ohm},c}$	600 K	[27]
$a_{\text{ohm},e}$	$0.00294 \times 10^{-3} \text{ k}\Omega \text{ cm}$	[27]
$b_{\text{ohm},e}$	$10,350 \text{ K}$	[27]
$a_{\text{ohm},i}$	$0.1256 \times 10^{-3} \text{ k}\Omega \text{ cm}$	[27]
$b_{\text{ohm},i}$	4690 K	[27]

The thicknesses of the different layers (δ) and the constants a_{ohm} and b_{ohm} used for calculating the temperature-dependent resistivity (ρ) are listed in Table 4.

3.2.2. Electrochemical model calibration

The electrochemical performance predicted by the model has been calibrated against experimental data. Because the model aims to represent the performance of 2nd generation SOFCs from Topsoe Fuel Cell A/S (TOFC) and Risø National Laboratory, published data for this SOFC have been used. The model has been calibrated against a polarisation curve (75-cell stack, $12 \times 12 \text{ cm}^2$, 800°C and fuelled with H_2 and N_2) published by Linderroth et al. in [28]. An active cell area of 81 cm^2 has been assumed. Both modelled and experimental data as well as the error relative to the experimental data are presented in Fig. 2. The calibration was done at atmospheric pressure.

The model shows excellent agreement with the experimental data above a current density of 100 mA cm^{-2} . A current density of 300 mA cm^{-2} was chosen to represent the SOFC load in the following results.

3.3. Micro gas turbine

Modelling of gas turbines is well described in the literature. The reader is referred to Saravanamuttoo et al. [29] for details. Characteristics of the turbomachinery and other components connected to the MGT are listed in Table 5.

The turbine inlet temperature (TIT) is limited to 900°C in the Gasifier–MGT case, while it varied in the Gasifier–SOFC–MGT arrangement. The performance of the compressors and the MGT expander corresponds to common performance data for an MGT of this scale, e.g., see [13]. The outlet pressure from the MGT depends on the total pressure loss downstream of the MGT because of the exhaust pressure, which is fixed at 1.013 bar. The outlet pressure from the MGT is slightly higher (1.033 bar) than the exhaust pressure due to the pressure drop in the recuperator and exhaust cooler.

3.4. Peripheral equipment

Modelling of peripheral components like heat exchangers is standard and therefore not described in detail.

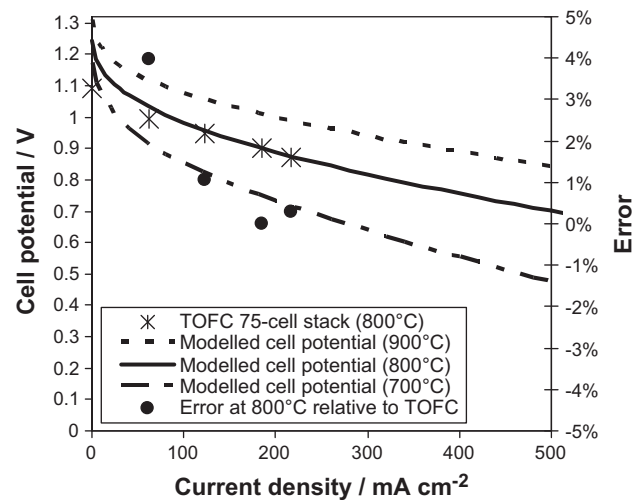


Fig. 2. Single cell polarisation curves based on a 75-cell stack at 800°C and the SOFC model, respectively. The modelled performance is shown for 700, 800 and 900°C and the relative error between the modelled and experimental performance is shown at 800°C .

Table 5

Inputs related to the MGT.

Isentropic efficiency of expander	84%
Isentropic efficiency of compressor	75%
Mechanical efficiency of compressor	98%
Maximum turbine inlet temperature ^a	900 °C
Recuperator effectiveness	85%
Generator efficiency	99%

^a Only an input in the Gasifier–MGT case.

The throughput of wet biomass is 154.8 kg h^{-1} (corresponds to $499.2 \text{ kW}_{\text{th}}$ (LHV)). Thus, it is assumed that the Viking gasifier can be scaled up from its nominal thermal input, which is $\sim 75 \text{ kW}_{\text{th}}$ [15]. The hot product gas preheats the ambient air for the gasifier from 15°C to 780°C before the syngas is used to dry the wet biomass. The biomass dryer reduces the water content in the biomass from 32.2 wt.% to 5 wt.% by heating it to 150°C . During the drying process, the biomass and hot syngas streams are separated. Because no drying component with separated streams exists in DNA, the modelling of this drying process is done by introducing a steam loop to transfer the heat from the syngas to the biomass as illustrated in Fig. 3. The superheated steam dries the biomass and the moisture from the biomass leaves the dryer together with the hot steam. The excess steam is separated from the steam loop and is exactly equal to the amount that evaporates from the biomass. No pressure losses are introduced in the steam loop and the steam blower is assumed to be ideal.

The gas cleaner is a bag filter that removes particulates and condensed impurities. It is assumed that the cleaned syngas can be directly used in an SOFC. The condenser removes some of the water from the syngas, resulting in a water content of 12.7 vol.% in the cleaned and dried syngas. The resulting steam to carbon ratio (S/C) is 0.41, which is somewhat low, but it is justified by the very low tar content in the Viking syngas.

The inlet temperatures to the SOFC anode and cathode are maintained at 150°C and 200°C below the outlet temperature, respectively. Thus, it is assumed that a cathode inlet temperature of 200°C lower than the SOFC operating temperature is possible.

The pressure loss in every component in the SOFC air supply stream and burner exhaust stream is assumed to be 10 mbar, whereas the pressure loss in each of the remaining components is assumed to be 5 mbar; the exception is the burner, which has a pressure loss of 0.6% (equals 1.5 mbar if 2.5 bar is present at the inlet). In [14], a pressure loss of 4.9 mbar is reported for the gas cleaner in the Viking gasifier, which fits well with the 5 mbar assumption used here.

The pressure ratio (defined over the air compressor) is different in the three scenarios; being close to 1 in the Gasifier–SOFC configuration, 3.7 in the Gasifier–MGT configuration and 2.5 in the Gas-

ifier–SOFC–MGT case. The pressure ratio is varied for the two pressurised systems as shown below.

No heat losses are taken into account. Introducing heat losses from the gas cleaner will only affect the heat production from the condenser because the temperature after the condenser is fixed at 50°C .

The district heating water is assumed to be 30°C at the inlet and 80°C at the outlet.

4. Results and discussion

In this section, the inputs presented in the previous sections are used unless otherwise stated. The different system configurations are described in detail in Section 2.

The performance of the different system configurations vary greatly with the operating conditions and the chosen pressure ratio

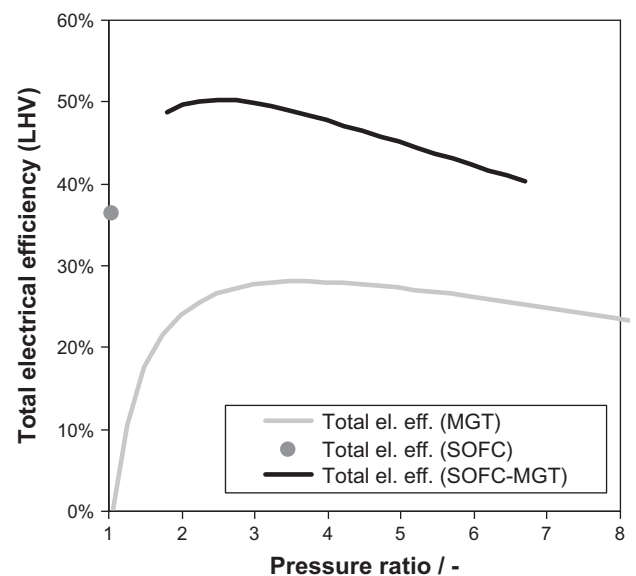


Fig. 4a. Energetic electric efficiency at different operating pressure ratios. The operating pressure ratio is defined over the air compressor.

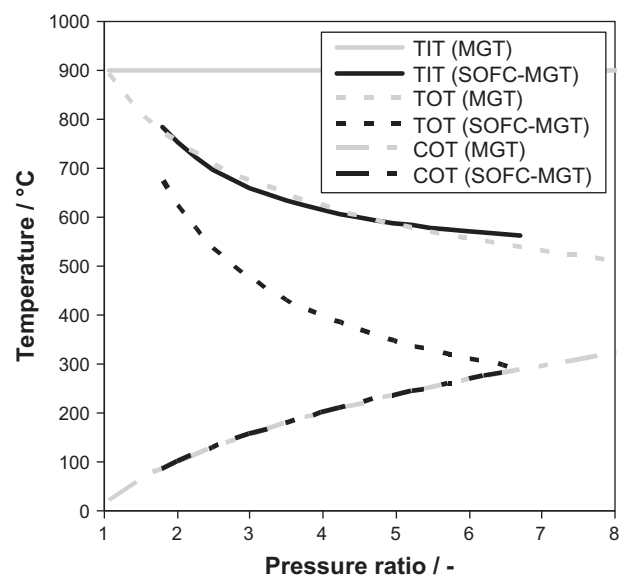


Fig. 4b. Turbine inlet temperature (TIT), turbine outlet temperature (TOT) and air compressor outlet temperature (COT) at different operating pressure ratios. Only the two pressurised system scenarios are illustrated.

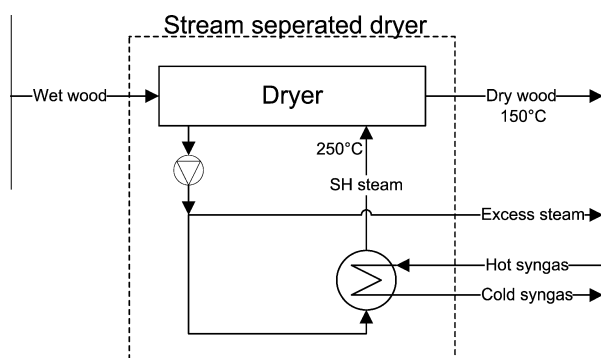


Fig. 3. Layout of the modelled dryer.

is of great importance to the resulting system performance. The different system configurations have different optima with regard to this operating pressure ratio. This relationship can be seen in Fig. 4a. In Fig. 4b, the corresponding turbine inlet temperatures (TIT), turbine outlet temperatures (TOT) and air compressor outlet temperatures (COT) are shown. When operating at a constant TIT of 900 °C, the Gasifier–MGT configuration shows an optimum at a pressure ratio of 3.7, performing with an electric efficiency of 28.1% (energetic and based on LHV). The recuperator ensures an optimum at a relatively low pressure ratio. Obviously, the pressure in the Gasifier–SOFC case is constantly near atmospheric pressure. This system performs at an electrical efficiency of 36.4%. The Gasifier–SOFC configuration has a higher efficiency because conversion in the SOFC is more efficient than that in the MGT, but the SOFC cannot utilise all of the fuel. With a fuel utilisation rate of 85%, a substantial portion of the fuel passes through the anode and is converted to heat in the burner. By combining the SOFC and MGT in the Gasifier–SOFC–MGT configuration, this heat can be used for further electricity production. At the optimum operating pressure ratio of 2.5, the combined system configuration reaches an electrical efficiency of 50.3%, thereby outperforming the two simpler configurations. The substantial increase in efficiency is mainly the result of better utilisation of unconverted fuel from the SOFC, but it is also due to the pressurised operation of the SOFC.

In the Gasifier–SOFC–MGT arrangement, the TIT decreases with an increasing pressure ratio. This relationship is due to the fact that an increasing PR increases the COT and reduces the TOT, which means that less heat is transferred in the recuperator. Therefore, more heat must be transferred in the SOFC air preheater to reach the same cathode inlet temperature. More heat transfer in the SOFC air preheater results in a lower temperature of the cathode off gas fed to the burner, thus decreasing the TIT. Furthermore, the TIT is lower in the Gasifier–SOFC–MGT case compared to the Gasifier–MGT scenario because less fuel is used to produce heat. A TIT of 697 °C is reached at a PR = 2.5. The optimal PR is lower in the Gasifier–SOFC–MGT scenario relative to the Gasifier–MGT arrangement due to the lower TIT. Characteristically, lowering the TIT of a recuperated gas turbine will lower the optimal PR. The slight increase in the SOFC efficiency observed with increasing pressure is not sufficient to change the resulting electrical efficiency trend of the hybrid system. Note that above a PR of

approximately 6.7 in the Gasifier–SOFC–MGT case, the TOT becomes lower than the COT, making it impossible to use a recuperator. Below a PR = 1.8, the heat transfer in the recuperator is sufficiently high to heat the air above the desired cathode inlet temperature.

The Gasifier–MGT system performance is also dependent on the allowed TIT as depicted in Fig. 5. Decreasing the TIT by 100 °C to 800 °C lowers the electrical efficiency to 25.4% – a drop of 2.7 percentage points. Considering the Gasifier–SOFC case, the sensitivity to the SOFC operating temperature is even greater. Lowering the SOFC operating temperature by 100 °C to 700 °C decreases the electrical efficiency to 28.8% – a drop of 7.6 percentage points. This differential effect indicates that the SOFC operating temperature has a greater influence on SOFC performance than the TIT has on MGT performance. In the Gasifier–SOFC–MGT configuration, a drop in the SOFC operating temperature by 100–700 °C decreases the electrical efficiency to 44.4% – a drop of 5.9 percentage points. The resulting TIT in the Gasifier–SOFC–MGT scenario shows dampened sensitivity to the chosen SOFC operating temperature because the SOFC air and fuel preheaters transfer more heat at higher SOFC operating temperatures to ensure maintenance of the temperature gradients across the anode and cathode. Therefore, temperatures of the SOFC off gases fed to the burner are not significantly affected by variation of the SOFC operating temperature.

The progress in research and development aimed at lowering the SOFC operating temperature may facilitate the use of cheaper materials, but will also influence system performance. If this is the case, other bottoming cycles could be beneficial, e.g., a Rankine cycle. An MGT development that allows for a higher TIT and an SOFC development that enables lowering of the SOFC temperature could lessen the gap between the electrical efficiencies of the Gasifier–MGT and the Gasifier–SOFC configurations.

An important aspect of SOFC systems is SOFC cooling. Given that the SOFC inlet and outlet temperatures are fixed, air flow through the cathode is determined by the cooling requirement of the SOFC in order to maintain a certain operating temperature. In Fig. 6, the cathode inlet temperature is varied. It is equivalent to changing the temperature gradient across the cathode (ΔT_c). A higher inlet temperature (a lower ΔT_c) decreases the electrical efficiency of the system. This effect is more pronounced in the Gasifier–SOFC–MGT configuration than in the Gasifier–SOFC configuration. An increase in the cathode inlet temperature from 600 to

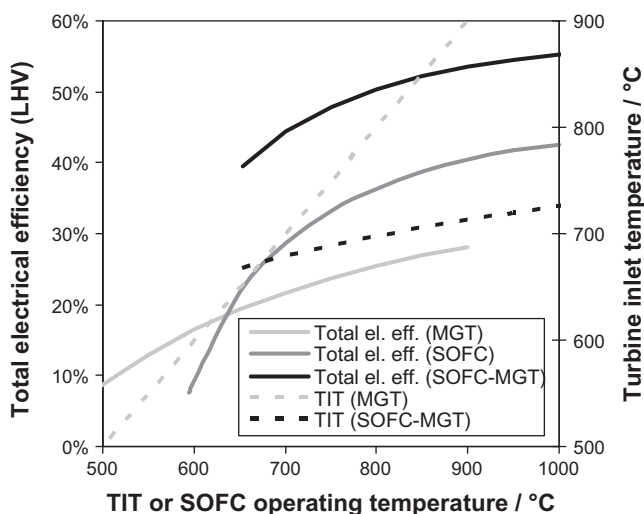


Fig. 5. Energetic electric efficiency and TIT at different TIT or SOFC operating temperatures. The TIT in the Gasifier–MGT case is defined at the gas turbine inlet and the SOFC operating temperature in the two other configurations is defined at the anode/cathode outlets. The maximum allowed TIT is 900 °C.

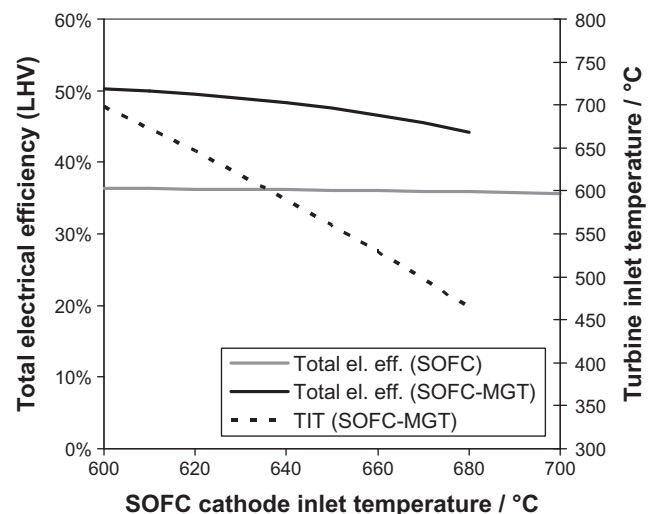


Fig. 6. Energetic electrical efficiency and TIT as a function of SOFC cathode inlet temperature.

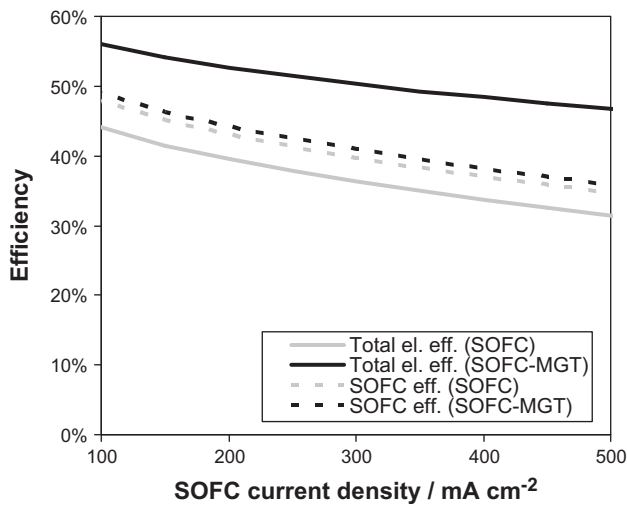


Fig. 7. System electrical efficiency and SOFC efficiency as a function of SOFC current density.

680 °C results in a decrease in the electrical efficiency of the Gasifier–SOFC–MGT arrangement from 50.3% to 44.1%, while it only

Table 6

Key data for the studied system configurations.

	Gasifier–MGT	Gasifier–SOFC	Gasifier–SOFC–MGT
Biomass throughput/kg h ^{−1}	154.8	154.8	154.8
Energetic biomass input/kW _{th} (LHV)	499.2	499.2	499.2
Exergetic biomass input ($ex_{biomass}$)/kW	572.4	572.4	572.4
Exergetic air input (ex_{air})/kW	6.6	6.6	6.6
PR/–	3.7	1.04	2.5
MGT net power production/kW _{el}	140.1	–	59.2
SOFC net power production/kW _{el}	–	181.5	191.8
Total net power production/kW _{el}	140.1	181.5	251.0
District heating production/kJ s ^{−1}	239.7	216.6	146.7
$\eta_{el}/\%$ (LHV)	28.1	36.4	50.3
$\eta_{CHP}/\%$ (LHV)	76.1	79.7	79.7
$\eta_{ex,el}/\%$ ^a	24.2	31.3	43.4
$\eta_{ex,CHP}/\%$ ^b	65.6	68.8	68.7

^a Defined as $\eta_{ex,el} = P_{net,tot}/(ex_{biomass} + ex_{air})$.

^b Defined as $\eta_{ex,CHP} = (P_{net,tot} + Q_{DH})/(ex_{biomass} + ex_{air})$.

drops from 36.4% to 35.9% in the Gasifier–SOFC configuration. In the Gasifier–SOFC scenario, the air compressor (working as a blower) consumes more power when the ΔT_c is decreased because a higher mass flow of air must be fed to the cathode to ensure a

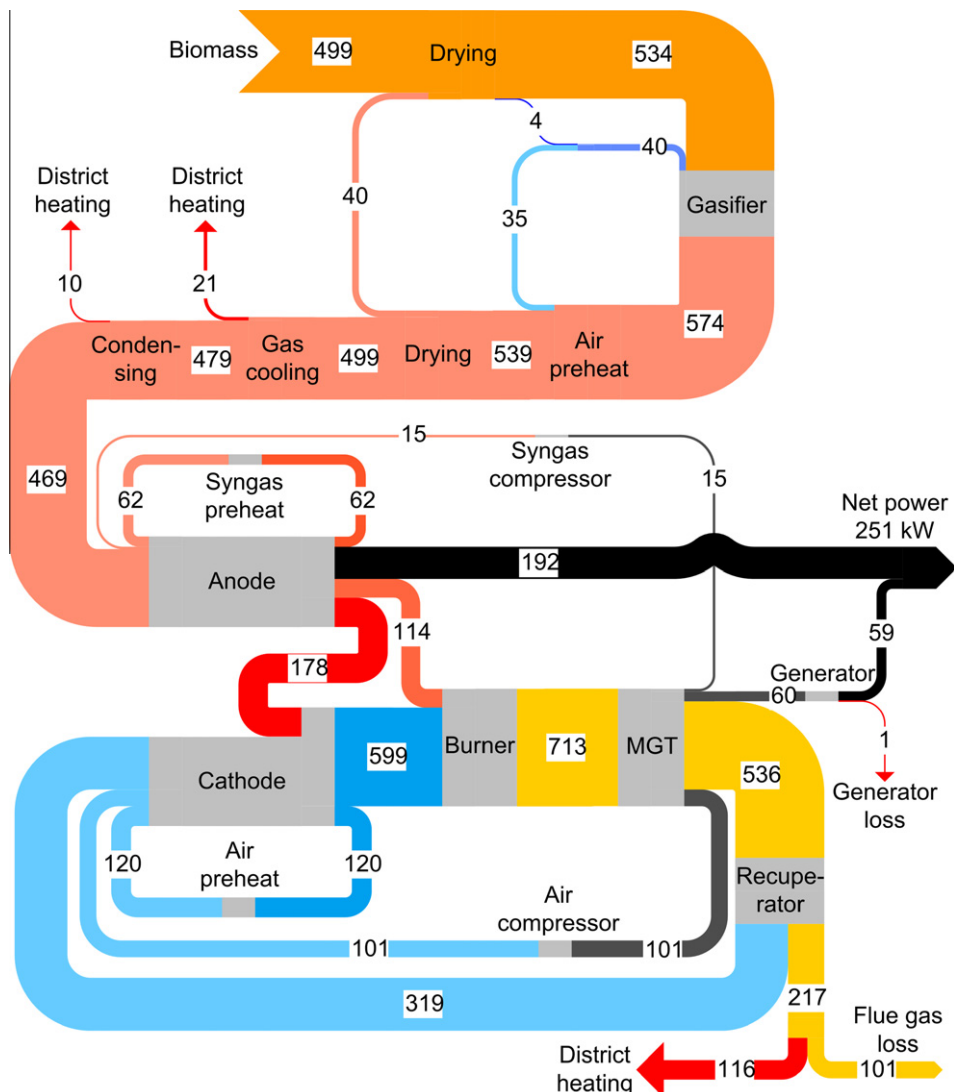


Fig. 8. Sankey diagram of the energy flows (rounded values in [kJ s^{−1}]) in the Gasifier–SOFC–MGT arrangement.

constant SOFC operating temperature. Thus, the parasitic losses increase, which in turn, slightly lower the electrical efficiency of the system. In the Gasifier–SOFC–MGT arrangement, the higher mass flow of air also passes through the MGT expander, thereby compensating for the greater air compressor work. The higher sensitivity to the chosen cathode inlet temperature in the Gasifier–SOFC–MGT scenario is explained by the following two facts: one, a lower ΔT_c results in a lower temperature of the cathode off gas fed to the burner (more heat transfer in the SOFC air preheater) and thus results in a lower TIT; and two, a lower ΔT_c necessitates a higher mass flow of air to maintain the same SOFC operating temperature, which ensures a more lean mixture in the burner and thereby decreases the TIT. Therefore, lowering the ΔT_c lowers the TIT, which decreases the MGT output and hence the electrical efficiency of the Gasifier–SOFC–MGT system.

The sensitivity of the model results to the chosen SOFC current density is shown in Fig. 7. At the reference current density value of 300 mA cm^{-2} , the total SOFC efficiency ($= \eta_{\text{rev}} \eta_v U_F$) is 39.6% in the Gasifier–SOFC arrangement and 40.8% in the Gasifier–SOFC–MGT case. The difference in SOFC efficiencies is due to the higher SOFC operating pressure in the Gasifier–SOFC–MGT case. Raising the SOFC load to 500 mA cm^{-2} reduces the SOFC efficiencies to 34.6% and 35.7% in the Gasifier–SOFC and Gasifier–SOFC–MGT cases, respectively. These decreases result in reductions in the total electrical efficiencies to 31.5% and 46.7%, respectively – equivalent to respective losses of 4.9% and 3.6 percentage points. These losses cause relative changes in electrical efficiency of 13.5% and 7.2%, respectively, for a 66.7% increase in current density. Therefore, the model is only moderately sensitive to the chosen current density. Furthermore, it is evident that a downstream MGT can raise the electrical efficiency of the total system above the performance of the SOFC alone. As mentioned earlier, this benefit is due to the utilisation of excess fuel from the SOFC.

Key data for the three studied system configurations are presented in Table 6. The respective optimal pressure ratio is used in each configuration as well as the reference input values presented in the previous sections. The Gasifier–SOFC–MGT configuration clearly has the best energetic- and exergetic-based electrical efficiency, while the CHP efficiencies do not significantly differ. In the Gasifier–SOFC–MGT case, power production is mainly derived from the SOFC, which produces 76.4% of the power. The exact efficiencies will be slightly lower when incorporating heat losses. Despite the neglected of heat losses, the comparisons of the systems' performances are still valid.

A Sankey diagram of the energy flows in the Gasifier–SOFC–MGT configuration is presented in Fig. 8. The Sankey diagram clearly shows the flow of energy, e.g. it clearly shows that heat is transferred from the anode to the cathode and that the flue gas loss from the exhaust of the hybrid system is approximately 100 kJ s^{-1} . In addition, it is evident that approximately 50% of the fuel is converted into electric power, while about 29% of it is used for district heating.

5. Conclusion

A study on the system performance of an up scaled Viking gasifier ($\sim 500 \text{ kW}_{\text{th}}$) with either a downstream MGT, SOFC or both has been conducted by process modelling combining zero-dimensional component models. An SOFC submodel has been developed, including an electrochemical model, which predicts the SOFC performance at different operating conditions. This submodel has been calibrated against published stack performance data from Topsoe Fuel Cell A/S.

For the two pressurised system configurations, the optimal operating pressure ratio was found to be 3.7 when using a recuper-

ated MGT and 2.5 when using an SOFC–MGT combination. Inclusion of an SOFC lowers the TIT (less fuel is converted to heat), thereby lowering the optimal pressure ratio. Operation of the syngas fuelled SOFC alone was performed at atmospheric pressure. The SOFC converted the syngas more efficiently than the MGT, which is reflected in the efficiency of the gasifier and MGT system configuration in opposition to the efficiency of the gasifier and SOFC configuration – $\eta_{\text{el}} = 28.1\%$ ($\eta_{\text{ex,el}} = 24.2\%$) versus $\eta_{\text{el}} = 36.4\%$ ($\eta_{\text{ex,el}} = 31.3\%$). Combining the two technologies achieved the highest efficiency of $\eta_{\text{el}} = 50.3\%$ ($\eta_{\text{ex,el}} = 43.4\%$) due to the efficient SOFC, utilisation of unconverted syngas from the SOFC in the MGT and pressurisation of the SOFC.

The calculated efficiencies were very sensitive to the chosen pressure ratio and SOFC operating temperature (or TIT in the Gasifier–MGT arrangement), whereas only moderate sensitivity to the temperature difference across the SOFC cathode and the SOFC current density was observed. From a system efficiency point of view, it is concluded that inclusion of an SOFC necessitates maintaining a high SOFC operating temperature and maximising the cathode temperature gradient and that inclusion of a recuperated MGT permits determination of the optimal pressure ratio.

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Appendix H PAPER II

Proceedings Paper - Peer Reviewed Manuscript

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MODELLING A COMBINED HEAT AND POWER PLANT BASED ON GASIFICATION, MICRO GAS TURBINE AND SOLID OXIDE FUEL CELLS

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ABSTRACT

A system level modelling study on two combined heat and power (CHP) systems both based on biomass gasification. One system converts the product gas in a micro gas turbine (MGT) and the other in a combined solid oxide fuel cell (SOFC) and MGT arrangement. An electrochemical model of the SOFC has been developed and calibrated against published data from Topsoe Fuel Cells A/S (TOFC) and Risø National Laboratory, and the modelled gasifier is based on an up scaled version of the demonstrated low tar gasifier, Viking, situated at the Technical University of Denmark. The SOFC converts the syngas more efficient than the MGT reflected in the electrical efficiency of the gasifier and MGT system in opposition to the gasifier and SOFC-MGT configuration - $\eta_{el}=28.1\%$ versus $\eta_{el}=50.3\%$.

Keywords: System modelling, biomass gasification, micro gas turbine, SOFC

NOMENCLATURE

a_{ohm}, b_{ohm}	coefficients for Eq. (24)
ASR	area specific resistance
E	reversible open circuit voltage
F	Faradays constant
g_f	Gibbs free energy of formation
i	current density
LHV	lower heating value
\dot{n}	molar flow
n_e	transferred electrons per molecule of fuel
p	pressure/partial pressure
P	power production
R	universal gas constant
T	temperature
UF	fuel utilization factor for SOFC
V	potential/overpotential
y	molar fraction
δ	SOFC layer thickness
η	efficiency

Subscripts:

a	anode
c	cathode
con	consumption
e	electrolyte
i	interconnect

INTRODUCTION

Development of sustainable and efficient production plants of combined heat and power (CHP) tends to gain more attention as climate changes, security of supply and depletion of fossil fuels have become well known issues. The share of biomass in CHP production are expected to increase in the future and decentralized CHP plants are also of interest to avoid costs of biomass transportation. Efficient power producing technologies for small scale productions are typically gas engines, micro gas turbines (MGT) and fuel cells – all requiring gaseous fuel. Gasification can deliver biomass based gaseous fuel so the combination of biomass gasification and efficient syngas conversion are potentially a sustainable and efficient CHP plant.

Solid oxide fuel cells (SOFCs) can electrochemically convert H_2 and CO as well as internally reform CH_4 into more H_2 and CO due to their high operating temperature. This makes SOFCs very fuel flexible and ideal for converting syngas compared to other fuel cell types.

The performance and system design of integrated biomass gasifier and SOFC systems in the 100-

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This study focus on the performance of a system combining an up scaled version ($\sim 500\text{kW}_{\text{th}}$) of the two-stage gasifier named Viking and a MGT or a SOFC-MGT system. Viking is a 75kW_{th} auto-thermal (air blown) fixed bed biomass gasifier demonstrated at the Technical University of Denmark and it is described in detail in [3]. The Viking gasifier produces almost no tars, which is favourable for downstream SOFC operation. Hofmann et al. [4] has operated a SOFC on cleaned syngas from the Viking gasifier for 150 hours without degradation.

SYSTEM DESCRIPTION

SOFC-MGT configuration, respectively. In the Gasifier-SOFC-MGT configuration all the components in the flow sheet are in use. With respect to Figure 1 the SOFC and preheaters are bypassed in the Gasifier-MGT arrangement. In addition the syngas compressor works as a roots blower for the gasifier system and not illustrated is a generator.

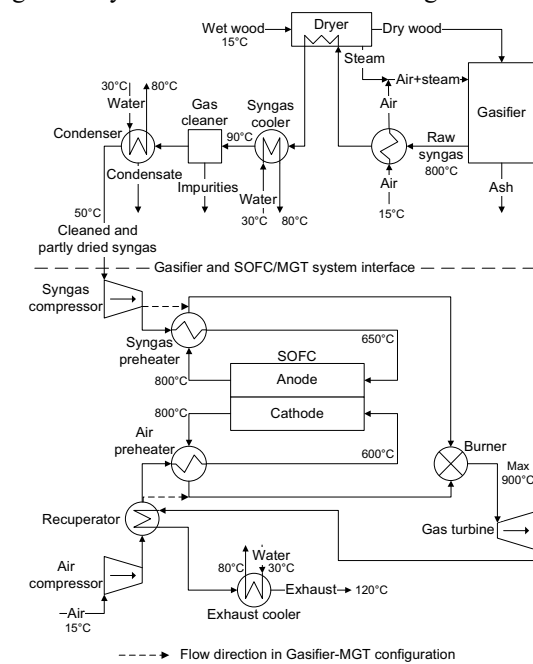


Figure 1: Flow sheet of the hybrid systems

Operating pressure	p_{gasifier}	0.998 bar
Operating temperature	T_{gasifier}	800°C
Pressure loss	$\Delta p_{\text{gasifier}}$	5 mbar
Non-equilibrium methane	$METH$	0.01

Table 1: Inputs to the gasifier submodel

GASIFIER MODEL

The gasifier component calculates the produced syngas composition as well as the produced ashes based on the inlet media composition and the operating conditions. The input parameters defining the operating conditions for the gasifier submodel are given in Table 1. The gasifier pressure loss is defined as the difference between the inlet air and steam mixture and the outlet syngas.

In the gasifier the incoming flows are converted into a syngas and ashes. The ashes come from a defined content in the biomass. The syngas can consist of the following species: H_2 , O_2 , N_2 , CO ,

NO, CO₂, H₂O, NH₃, H₂S, SO₂, CH₄, NO₂, HCN, COS and Ar. It is assumed that equilibrium is reached at the operating temperature and pressure, where the total Gibbs energy has its minimum value. With this assumption the syngas outlet composition can be found by the Gibbs minimization method [6]. A possibility for bypassing an amount of methane from the equilibrium calculations is added in order to reach syngas compositions, which contain more methane than the corresponding one at equilibrium. Thus the syngas composition can be adjusted to match real syngas compositions, e.g. from the Viking gasifier. The input parameter *METH* is used for this bypassing and is defined as the fraction of the methane that is not included in the equilibrium calculations and instead flows through the gasifier and appears in the outlet syngas.

Gasifier model validation

The model validation for the gasifier is done for all of the gasification plant from the biomass input to the cleaned and dried syngas. Thus the data from the Viking gasifier plant can be used for validation.

Wood chips from beech with small amounts of oak are used in the modelling as for the Viking gasifier reported in Ahrenfeldt et al. [3].

As seen in Table 2 the produced syngas composition and the lower heating value (LHV) from the gasifier model is close to the Viking data. The overall performance of the modelled gasifier is also similar to the Viking gasifier expressed in the cold gas efficiencies.

SOLID OXIDE FUEL CELL MODEL

The SOFC stack component calculates the air and fuel outlet compositions as well as the power production. The calculations are based on the inlet air and fuel compositions and flow rates as well as the other operating conditions of the SOFC. The SOFC submodel includes an electrochemical model for predicting the performance of the SOFC. The operating conditions are partly described by input parameters given to the SOFC submodel and these are presented in Table 3.

In the submodel only H₂ is electrochemically converted in the SOFC anode, but the model takes into account that CO produces an extra H₂ through

	Viking [3]	Gasifier model
H ₂ (vol-%)	30.5	29.9
CO (vol-%)	19.6	20.8
CO ₂ (vol-%)	15.4	13.5
CH ₄ (vol-%)	1.16	1.19
N ₂ (vol-%)	33.3	34.2
LHV (MJ/kg)	6.2	6.3
Cold gas eff.	93%	94%

Table 2: Dry syngas composition, lower heating value as well as cold gas efficiency for the Viking gasifier and the modelled gasifier, respectively

Fuel utilization factor	UF	0.85
Operating temperature	T_{SOFC}	800°C
Anode pressure loss	Δp_a	5 mbar
Cathode pressure loss	Δp_c	10 mbar
Current density	i	300 mA cm ⁻²

Table 3: Inputs to the SOFC submodel

the water-gas-shift (WGS) reaction, while four additional H₂ molecules are produced from CH₄ through internal steam reforming and WGS of produced CO (full conversion is assumed). The total mole flow of H₂ on the anode after internal steam reforming and WGS is expressed in Eq. (1).

$$\dot{n}_{H_2, \text{tot}} = \dot{n}_{H_2, \text{in}} + \dot{n}_{CO, \text{in}} + 4\dot{n}_{CH_4, \text{in}} \quad (1)$$



The amount of hydrogen that is converted depends on the fuel utilization factor (UF) and this amount is electrochemically converted in the anode. The electrode reactions and the overall fuel cell reaction are as shown in Eq. (2) to (4).

From the overall fuel cell reaction it is seen that the amount of consumed oxygen is half the amount of consumed hydrogen. The cathode outlet composition can then be found by the following equations if the only species taking into account are O₂, N₂, CO₂, H₂O and Ar.

$$\dot{n}_{O_2, \text{con}} = \frac{UF\dot{n}_{H_2, \text{in}}}{2} \quad (5)$$

$$\dot{n}_{c, \text{out}} = \dot{n}_{c, \text{in}} - \dot{n}_{O_2, \text{con}} \quad (6)$$

$$y_{O_2,out} = \frac{\dot{n}_{c,in} y_{O_2,in} - \dot{n}_{O_2,con}}{\dot{n}_{c,out}} \quad (7)$$

$$y_{j,out} = \frac{\dot{n}_{c,in} y_{j,in}}{\dot{n}_{c,out}}, \quad j = \{N_2, CO_2, H_2O\} \quad (8)$$

$$y_{Ar,out} = 1 - y_{O_2,out} - y_{N_2,out} - y_{CO_2,out} - y_{H_2O,out} \quad (9)$$

The fuel composition leaving the anode is calculated by the Gibbs minimization method [6] as described for the gasifier submodel. Equilibrium at the anode outlet temperature and pressure is assumed for the following species: H_2 , CO , CO_2 , H_2O , CH_4 and N_2 . The equilibrium assumption is fair since the methane content in this study is low enough for such kind of assumption to be made. The heat consumed by the endothermic internal reforming reactions is taken into account by the Gibbs minimization method. More internal reforming means more cooling of the SOFC.

The power production from the SOFC depends on the amount of chemical energy fed to the anode, the reversible efficiency (η_{rev}), the voltage efficiency (η_v) and the fuel utilization factor (UF). It is defined in mathematical form in Eq. (10).

$$P_{SOFC} = \left[\begin{array}{l} LHV_{H_2} \dot{n}_{H_2,in} \\ + LHV_{CO} \dot{n}_{CO,in} \\ + LHV_{CH_4} \dot{n}_{CH_4,in} \end{array} \right] \eta_{rev} \eta_v UF \quad (10)$$

The reversible efficiency is the maximum possible efficiency defined as the relationship between the maximum electrical energy available (change in Gibbs free energy) and the fuels LHV. This is shown in Eq. (11) and the definition of the change in Gibbs free energy is shown in Eq. (12). The voltage efficiency express the electrochemical performance of the SOFC and the calculation of the voltage efficiency is described in the following subsection.

$$\eta_{rev} = \frac{(\Delta \bar{g}_f)_{fuel}}{LHV_{fuel}} \quad (11)$$

$$\begin{aligned} (\Delta \bar{g}_f)_{fuel} = & \left[(\bar{g}_f)_{H_2O} - (\bar{g}_f)_{H_2} - \frac{1}{2} (\bar{g}_f)_{O_2} \right] y_{H_2,in} \\ & + \left[(\bar{g}_f)_{CO_2} - (\bar{g}_f)_{CO} - \frac{1}{2} (\bar{g}_f)_{O_2} \right] y_{CO,in} \\ & + \left[(\bar{g}_f)_{CO_2} + 2(\bar{g}_f)_{H_2O} - (\bar{g}_f)_{CH_4} - 2(\bar{g}_f)_{O_2} \right] y_{CH_4,in} \end{aligned} \quad (12)$$

Electrochemical model

The electrochemical model is used to calculate the cell potential and the voltage efficiency of the SOFC. Both depend on the operating conditions such as temperature, pressure, gas compositions, fuel utilization and load (current density). The cell potential and voltage efficiency is defined in Eq. (13) and (14), respectively.

$$V_{cell} = E - V_{act} - V_{ohm} \quad (13)$$

$$\eta_v = \frac{V_{cell}}{E} \quad (14)$$

In the following the reversible open circuit voltage (E), the activation overpotential (V_{act}) and the ohmic overpotential (V_{ohm}) are calculated. Traditionally a concentration overpotential term is included in Eq. (13). The concentration overpotential is a result of the limitations of transporting the reactants to the active cell area. In Larminie et. al. [7] it is described as a voltage drop caused by the pressure change associated with the consumption of reactants. As a result of the current being drawn from the cell the average partial pressure of reactants is lower than at the inlet. Thus, in this study the concentration overvoltage is taken into account by using average partial pressures when calculating E and V_{act} .

E can be calculated from the Nernst equation:

$$E = \frac{-\Delta \bar{g}_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{\bar{p}_{H_2,tot} \sqrt{\bar{p}_{O_2}}}{\bar{p}_{H_2O}} \right) \quad (15)$$

Since it is assumed that all CO and CH_4 are converted to H_2 before the electrochemical reactions takes place, the change in standard Gibbs free energy ($\Delta \bar{g}_f^0$) and the number of electrons transferred for each molecule of fuel (n_e) is determined for the reaction of H_2 only. Thus, $n_e = 2$ and $\Delta \bar{g}_f^0 = (\bar{g}_f^0)_{H_2O} - (\bar{g}_f^0)_{H_2} - \frac{1}{2} (\bar{g}_f^0)_{O_2}$. The partial pressure of species j is an average across the respective electrode and is here defined as an arithmetic mean between inlet and outlet as shown in Eq. (16) and (17). The average partial pressure of available hydrogen after internal steam reforming and WGS of CH_4 and CO can be determined from

the overall steam reforming and WGS reaction including all species. It is defined in Eq. (18):

$$\bar{p}_j = \left(\frac{y_{j,\text{out}} - y_{j,\text{in}}}{2} \right) p_a, \quad (16)$$

$$j = \{H_2, CO, CH_4, CO_2, H_2O, N_2\}$$

$$\bar{p}_{O_2} = \left(\frac{y_{O_2,\text{out}} - y_{O_2,\text{in}}}{2} \right) p_c \quad (17)$$

$$\bar{p}_{H_2,\text{tot}} = \left(\frac{\bar{p}_{H_2} + \bar{p}_{CO} + 4\bar{p}_{CH_4}}{\bar{p}_{H_2} + \bar{p}_{CO} + 3\bar{p}_{CH_4} + \bar{p}_{CO_2} + \bar{p}_{H_2O} + \bar{p}_{N_2}} \right) p_a \quad (18)$$

The activation overpotential is due to an energy barrier (activation energy) that the reactants must overcome in order to drive the electrochemical reactions. The activation overpotential is non-linear and is dominant at low current density (i). The activation overpotential is defined as (cf. [8]):

$$\begin{aligned} V_{\text{act}} &= V_{\text{act},a} + V_{\text{act},c} \\ &= \frac{2RT}{n_e F} \left[\sinh^{-1} \left(\frac{i + i_n}{2i_{0,a}} \right) + \sinh^{-1} \left(\frac{i + i_n}{2i_{0,c}} \right) \right] \end{aligned} \quad (19)$$

The internal current density (i_n) is added to the actual fuel cell current density in order to account for the mixed potential caused by fuel crossover. The importance of the internal current density in the case of SOFCs is much less than for low temperature fuel cells and the value of i_n is usually very small [7]. The exchange current density (i_0) is a measure of the level of activity on the electrode at $i=0 \text{ mA cm}^{-2}$ and is defined as (cf. [9]):

$$i_{0,a} = 2.13 \times 10^7 \left(\frac{\bar{p}_{H_2,\text{tot}} \bar{p}_{H_2O}}{p_a^2} \right) \exp \left(\frac{-110000}{RT} \right) \quad (20)$$

$$i_{0,c} = 1.49 \times 10^7 \left(\frac{\bar{p}_{O_2}}{p_c} \right)^{0.25} \exp \left(\frac{-110000}{RT} \right) \quad (21)$$

The ohmic overpotential is caused by the electrical resistance for the ions passing through the electrolyte as well as for the electrons passing through the electrodes and interconnects. The

R	$8.314 \text{ J K}^{-1} \text{ mol}^{-1}$
F	96485 C mol^{-1}
n_e	2
i_n	2 mA cm^{-2} [9]
δ_a	$750 \times 10^{-4} \text{ cm}$ [10]
δ_c	$50 \times 10^{-4} \text{ cm}$ [10]
δ_e	$40 \times 10^{-4} \text{ cm}$ [10]
δ_i	$100 \times 10^{-4} \text{ cm}$ [11]
$a_{\text{ohm},a}$	$0.00298 \times 10^{-3} \text{ k}\Omega \text{ cm}$ [12]
$b_{\text{ohm},a}$	-1392 K [12]
$a_{\text{ohm},c}$	$0.00811 \times 10^{-3} \text{ k}\Omega \text{ cm}$ [12]
$b_{\text{ohm},c}$	600 K [12]
$a_{\text{ohm},e}$	$0.00294 \times 10^{-3} \text{ k}\Omega \text{ cm}$ [12]
$b_{\text{ohm},e}$	10350 K [12]
$a_{\text{ohm},i}$	$0.1256 \times 10^{-3} \text{ k}\Omega \text{ cm}$ [12]
$b_{\text{ohm},i}$	4690 K [12]

Table 4: Inputs for the electrochemical model

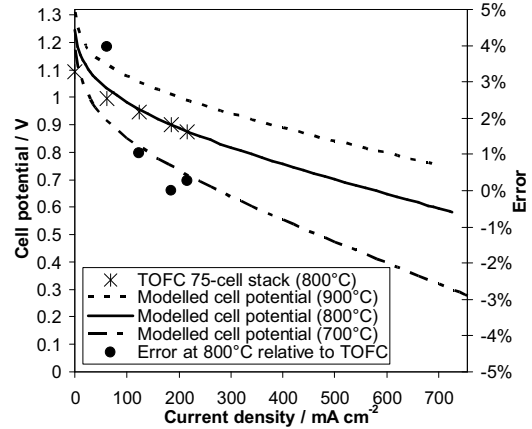


Figure 2: Single cell polarization curves based on a 75-cell stack and the SOFC model, respectively.

ohmic overpotential is defined below (cf. [9] and [12]).

$$V_{\text{ohm}} = i ASR \quad (22)$$

$$ASR = ASR_a + ASR_c + ASR_e + ASR_i \quad (23)$$

$$ASR_j = \delta_j a_{\text{ohm},j} \exp \left(\frac{b_{\text{ohm},j}}{T} \right), \quad j = \{a, c, e, i\} \quad (24)$$

The thicknesses of the different layers (δ) and the constants a_{ohm} and b_{ohm} used are listed in Table 4.

SOFC model calibration

The described electrochemical model has been calibrated against experimental data. Since the model aims at the performance of 2nd generation SOFCs from Topsoe Fuel Cell A/S (TOFC) and Risø National Laboratory, published data from this SOFC type has been used. The *ASR* has been calibrated against a value of $0.15 \Omega \text{ cm}^2$ at 850°C as published by [13] and the resulting cell potential has been calibrated against a polarization curve (800°C and fuelled with H_2 and N_2) published by [14]. An active cell area of 81 cm^2 has been assumed. Both modelled and experimental data as well as the error relative to the experimental data are presented in Figure 2.

The model shows excellent agreement with the experimental data above a current density of 100 mA cm^{-2} . The current density of 300 mA cm^{-2} is chosen to represent the SOFC load in the following results.

PERIPHERAL EQUIPMENT

Modelling of peripheral components like compressors, turbines and heat exchangers are standard and therefore not described in detail.

The throughput of wet biomass is 154.8 kg h^{-1} (corresponds to $499.2 \text{ kW}_{\text{th}}$ (LHV)). Thus it is assumed that the Viking gasifier can be scaled up from a nominal $\sim 75 \text{ kW}_{\text{th}}$ [3]. The biomass dryer reduces the water content in the biomass from 32.2 wt-% to 5 wt-% by heating it to 150°C and the air for the gasifier is preheated to 780°C by the hot product gas.

The inlet temperature to the SOFC anode and cathode are maintained at 150°C and 200°C below the outlet temperature, respectively.

The pressure loss in every component in the SOFC air supply stream and burner exhaust stream is assumed to be 10 mbar, while the pressure loss in each of the rest of the components is assumed to be 5 mbar, except the burner that has a pressure loss of 0.6% (equals 1.5 mbar when 2.5 bar at inlet).

The gas cleaner is a baghouse filter removing particulates and it is assumed that the cleaned syngas can be used directly in a SOFC. The condenser removes some of the water content in the syngas resulting in a content of water in the cleaned and dried syngas of 12.7 vol-%. The re-

sulting steam to carbon ratio (S/C) is 0.41, which is somewhat low, but is justified by the very low tar content in the Viking syngas.

The isentropic and mechanical efficiency of the compressors are 75% and 98%, respectively, and the isentropic efficiency of the MGT expander is 84%. The turbine inlet temperature (TIT) is limited to 900°C in the Gasifier-MGT case, while varied in the Gasifier-SOFC-MGT arrangement. The performance of the compressors and the MGT expander are taken from Fryda et al. [2] and corresponds to common performance data for a MGT of this scale. The recuperator effectiveness is assumed to be 85% and the generator efficiency is assumed to be 99%. In the Gasifier-MGT configuration the burner operating pressure is 3.75 bar and in the Gasifier-SOFC-MGT case the SOFC operating pressure is 2.5 bar (these pressures are varied in the results section).

No heat losses are taken into account. Introducing heat losses from the gas cleaner will only affect the heat production from the condenser since the temperature after the condenser is fixed to 50°C .

The outlet pressure from the MGT depends on the total pressure loss downstream the MGT, since it is the exhaust pressure which is fixed to 1.013 bar. Because of the recuperator and exhaust cooler the outlet pressure from the MGT is 1.033 bar. The district heating (DH) water is assumed to be 30°C at inlet and 80°C at outlet.

RESULTS AND DISCUSSION

In the following results the inputs presented in the previous sections are used unless something else is stated. The system configurations are previously described in detail.

The performance of the different system configurations vary greatly with the operating conditions and namely the pressure ratio of the MGT (in the Gasifier-MGT case) and the operating pressure of the SOFC (in the Gasifier-SOFC-MGT case) are of great importance to the resulting system performance. The two system configurations have different optimum with regard to their operating pressure and these can be seen in Figure 3. When operating at a constant TIT of 900°C the Gasifier-MGT configuration shows an optimum at 3.75 bar performing an electric efficiency of 28.1%. It is the recuperator that ensures an optimum at a rela-

tively low operating pressure. By combining the SOFC and MGT in the Gasifier-SOFC-MGT configuration the electrical efficiency reaches 50.3% at an optimum operating pressure of 2.5 bar. This is a substantial increase in efficiency caused by the efficient SOFC. With a fuel utilization of 85% a part of the fuel passes through the anode, but this amount is used in the MGT. In this case the TIT is varying with the SOFC operating pressure and has a value of 697°C at 2.5 bar.

The Gasifier-MGT system performance also depend on the allowed TIT as depicted in Figure 4. Decreasing the TIT by 100°C to 800°C lowers the electrical efficiency to 25.4% - a drop of 2.7 percentage points. In the Gasifier-SOFC-MGT configuration a drop in SOFC operating temperature by 100°C to 700°C decreases the electrical efficiency to 44.4% - a drop of 5.9 percentage points. This indicates that the SOFC operating temperature has more influence on the SOFC performance than the TIT has on the MGT performance. The research and development working on lowering the SOFC operating temperature in order to use cheaper materials will influence the system performance presented here and potentially other bottoming cycles could be beneficial, e.g. a Rankine cycle.

The sensitivity of the model results to the chosen SOFC current density is shown in Figure 5. At the reference current density value of 300 mA cm⁻² the SOFC voltage efficiency (defined in Eq. (14)) is 40.8%. Raising the SOFC load to 500 mA cm⁻² lowers the voltage efficiency to 35.7% meaning a reduction in the total electrical efficiency to 46.7% - a drop of 3.6 percentage points. This is a relative change in electrical efficiency of 7% for a 66.7% increase in current density.

Key data for the two system configurations studied are presented in Table 5 and the respective optimal operating pressure is used in each configuration as well as the reference input values presented in the previous sections. The Gasifier-SOFC-MGT configuration clearly has the best electrical efficiency, while the CHP efficiencies do not differ significantly. In the Gasifier-SOFC-MGT case, the power production is mainly from the SOFC producing 76.4% of the power. The exact values of the efficiencies will be slightly lower when incorporating heat losses, a more

accurate efficiency of the gasifier system and possible more extensive gas cleaning, but the comparison of the systems performance is still valid.

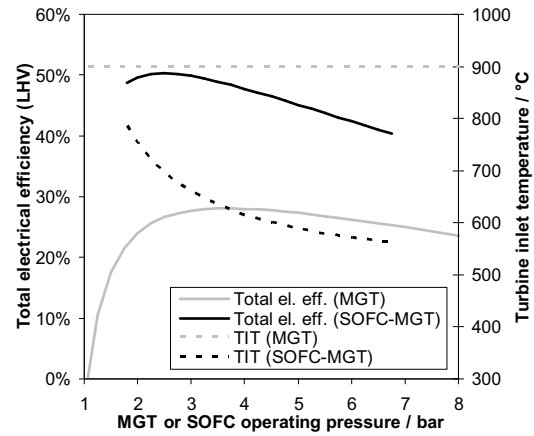


Figure 3: Electric efficiency and TIT at different MGT or SOFC operating pressures

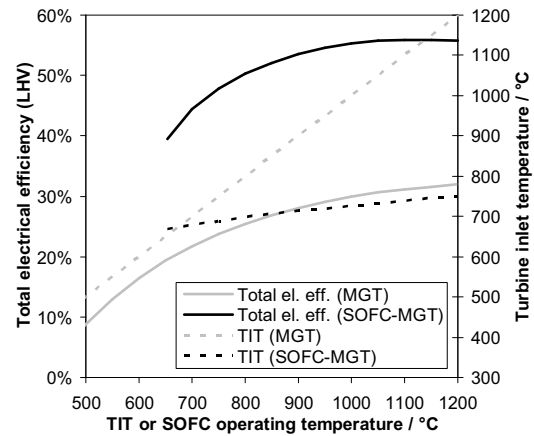


Figure 4: Electric efficiency and TIT at different TIT or SOFC operating temperatures

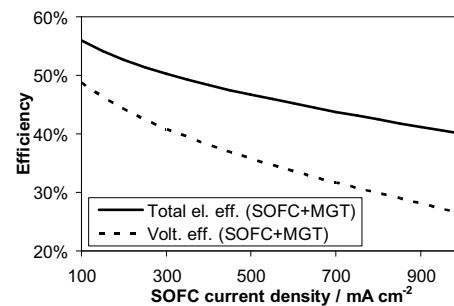


Figure 5: Electrical efficiency and SOFC voltage efficiency as a function of SOFC current density

		Gasifier -MGT	Gasifier -SOFC-MGT
Biomass input	/ kg h ⁻¹	154.8	154.8
	/ kW _{th,LHV}	499.2	499.2
p_{MGT} or p_{SOFC} / bar		3.75	2.5
$P_{\text{MGT,net}}$ / kW _{el}		140.1	59.2
$P_{\text{SOFC,net}}$ / kW _{el}		-	191.8
$P_{\text{total,net}}$ / kW _{el}		140.1	251.0
DH production / kJ s ⁻¹		239.7	146.7
η_{el} / % (LHV)		28.1	50.3
η_{CHP} / % (LHV)		76.1	79.7

Table 5: Key data for the studied systems

CONCLUSION

A study on the system performance of an up scaled Viking gasifier (~500 kW_{th}) with either a downstream MGT or SOFC-MGT has been conducted by zero dimensional process modelling. A SOFC submodel has been developed including an electrochemical model predicting the SOFC performance at different operating conditions. This submodel has been calibrated against published TOFC stack performance data. The reference conditions for the SOFC has been an operating temperature of 800°C, a fuel utilization of 85% and a current density of 300 mA cm⁻². The optimal operating MGT and SOFC-MGT pressure has been found for the two system configurations to 3.75 and 2.5 bar, respectively. The SOFC converted the syngas more efficient than the MGT reflected in the efficiency of the gasifier and MGT system configuration in opposition to the gasifier and SOFC-MGT configuration - η_{el} =28.1% versus η_{el} =50.3%. These efficiencies were very sensitive to the SOFC operating temperature (or TIT in the Gasifier-MGT arrangement), while only a moderate sensitivity to the SOFC current density was observed.

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Appendix I PAPER III

Proceedings Paper - Peer Reviewed Abstract

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Modelling of a Biomass Gasification Plant Feeding a Hybrid Solid Oxide Fuel Cell and Micro Gas Turbine System

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Abstract

A system level modelling study on two combined heat and power (CHP) systems both based on biomass gasification. One system converts the product gas in a solid oxide fuel cell (SOFC) and the other in a combined SOFC and micro gas turbine (MGT) arrangement. An electrochemical model of the SOFC has been developed and calibrated against published data from Topsoe Fuel Cells A/S (TOFC) and Risø National Laboratory. The modelled gasifier is based on an up scaled version of the demonstrated low tar gasifier, Viking, situated at the Technical University of Denmark. The MGT utilizes the unconverted syngas from the SOFC to produce more power as well as pressurizing the SOFC bettering the electrical efficiency compared to operation with the SOFC alone - from $\eta_{el}=36.4\%$ to $\eta_{el}=50.3\%$.

Keywords: System modelling, biomass gasification, micro gas turbine, SOFC

Nomenclature

a_{ohm}, b_{ohm}	coefficients for Eq. (24)
ASR	area specific resistance
E	reversible open circuit voltage
F	Faradays constant
g_f	Gibbs free energy of formation
i	current density
LHV	lower heating value
\dot{n}	molar flow
n_e	transferred electrons per molecule of fuel
p	pressure/partial pressure
P	power production
R	universal gas constant
T	temperature
UF	fuel utilization factor for SOFC
V	potential/overpotential
y	molar fraction
δ	SOFC layer thickness
η	efficiency

Subscripts:

a	anode
c	cathode
con	consumption
e	electrolyte
i	interconnect

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1 Introduction

Development of sustainable and efficient production plants of combined heat and power (CHP) tends to gain more attention as climate changes, security of supply and depletion of fossil fuels have become well known issues. The share of biomass in CHP production are expected to increase in the future and decentralized CHP plants are also of interest to avoid costs of biomass transportation. Efficient power producing technologies for small scale productions are typically gas engines, micro gas turbines (MGT) and fuel cells – all requiring gaseous fuel. Gasification can deliver biomass based gaseous fuel so the combination of biomass gasification and efficient syngas conversion are potentially a sustainable and efficient CHP plant.

Solid oxide fuel cells (SOFCs) can electrochemically convert H_2 and CO as well as internally reform CH_4 into more H_2 and CO due to their high operating temperature. This makes SOFCs very fuel flexible and ideal for converting syngas compared to other fuel cell types.

The performance and system design of integrated biomass gasifier and SOFC systems in the 100-1000kW_e class have been investigated by several. An innovative design including heat pipes between a SOFC stack and an allothermal gasifier is described in [1]. Fryda et al. [2] studies the performance of a CHP system of less than 1MW_e and consisting of an autothermal gasifier combined with a MGT and/or SOFC.

This study focus on the performance of a system combining an up scaled version (~500kW_{th}) of the two-stage gasifier named Viking and a SOFC or a SOFC-MGT system. Viking is a 75kW_{th} autothermal (air blown) fixed bed biomass gasifier demonstrated at the Technical University of Denmark and it is described in detail in [3]. The Viking gasifier produces almost no tars, which is favourable for downstream SOFC operation. Hofmann et al. [4] has operated a SOFC on cleaned syngas from the Viking gasifier for 150 hours without degradation.

The present study is based on zero dimensional and steady-state modelling in the simulation tool DNA [5]. DNA has incorporated thermodynamic property data, is component based and is developed at The Technical University of Denmark.

2 System description

Two different combined heat and power systems are investigated in this study, both based on syngas production from an up scaled Viking gasifier. A flow sheet of the two systems is depicted in Figure 1. The modelled gasifier system is slightly simplified, but aims at the same resulting gas composition and cold gas efficiency as for the Viking gasifier. In the gasifier model the dryer is heated by hot syngas. The steam production from the dryer is added to the preheated air and dry wood together with mixed air and steam are fed to the gasifier. The raw product gas is cooled to 90°C in three steps; air preheating, wood drying and syngas cooling producing hot water for district heating. The cooled syngas is then cleaned from impurities as particles and sulphur compounds before some of the water in the gas is condensed through cooling to 50°C. The cleaned and partly dried syngas is then converted into electricity and heat in a bottoming cycle consisting of a SOFC or both a SOFC and a MGT. These two system configurations will from now on be referred as the Gasifier-SOFC and the Gasifier-SOFC-MGT configuration, respectively. In the Gasifier-SOFC-MGT configuration all the components in the flow sheet are in use. With respect to Figure 1 the recuperator and gas turbine are bypassed in the Gasifier-SOFC arrangement, thus the syngas and air compressors work as blowers due to no pressurization. In addition the syngas compressor works as a roots blower for the gasifier system and not illustrated is a generator. In the Gasifier-SOFC configuration the syngas and air blowers are driven by an electric motor.

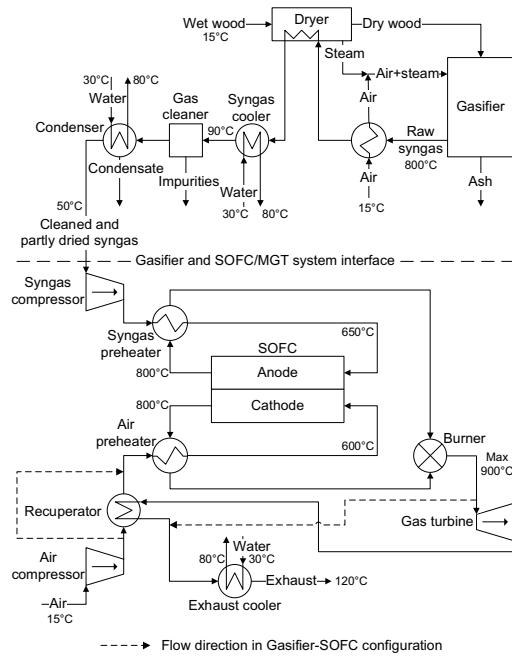


Figure 1: Flow sheet of the hybrid systems

3 Gasifier model

The gasifier component calculates the produced syngas composition as well as the produced ashes based on the inlet media composition and the operating conditions. The input parameters defining the operating conditions for the gasifier submodel are given in Table 1. The gasifier pressure loss is defined as the difference between the inlet air and steam mixture and the outlet syngas.

Operating pressure	p_{gasifier}	0.998 bar
Operating temperature	T_{gasifier}	800°C
Pressure loss	$\Delta p_{\text{gasifier}}$	5 mbar
Non-equilibrium methane	$METH$	0.01

Table 1: Inputs to the gasifier submodel

In the gasifier the incoming flows are converted into a syngas and ashes. The ashes come from a defined ash content in the biomass. The syngas can consist of the following species: H_2 , O_2 , N_2 , CO , NO , CO_2 , H_2O , NH_3 , H_2S , SO_2 , CH_4 , NO_2 , HCN , COS and Ar . It is assumed that equilibrium is reached at the operating temperature and pressure, where the total Gibbs energy has its minimum value. With this assumption the syngas outlet composition can be found by the Gibbs minimization method [6]. A possibility for bypassing an amount of methane from the equilibrium calculations is added in order to reach syngas compositions, which contain more methane than the corresponding one at equilibrium. Thus the syngas composition can be adjusted to match real syngas compositions, e.g. from the Viking gasifier. The input parameter $METH$ is used for this bypassing and is defined as the fraction of methane that is not included in the equilibrium calculations and instead flows through the gasifier and appears in the outlet syngas.

3.1 Gasifier model validation

The model validation for the gasifier is done for all of the gasification plant from the biomass input to the cleaned and dried syngas. Thus data from the Viking gasifier plant can be used for validation.

Wood chips from beech with small amounts of oak are used in the model as for the Viking gasifier reported in Ahrenfeldt et al. [3].

As seen in Table 2 the produced syngas composition and the lower heating value (LHV) from the gasifier model is close to the Viking data. The overall performance of the modelled gasifier is also similar to the Viking gasifier as expressed in the cold gas efficiencies.

	Viking [3]	Gasifier model
H ₂ (vol-%)	30.5	29.9
CO (vol-%)	19.6	20.8
CO ₂ (vol-%)	15.4	13.5
CH ₄ (vol-%)	1.16	1.19
N ₂ (vol-%)	33.3	34.2
LHV (MJ/kg)	6.2	6.3
Cold gas eff.	93%	94%

Table 2: Dry syngas composition, lower heating value as well as cold gas efficiency for the Viking gasifier and the modelled gasifier, respectively

4 Solid Oxide Fuel Cell model

The SOFC stack component calculates the air and fuel outlet compositions as well as the power production. The calculations are based on the inlet air and fuel compositions and flow rates as well as the other operating conditions of the SOFC. The SOFC submodel includes an electrochemical model for predicting the performance of the SOFC. The operating conditions are partly described by input parameters given to the SOFC submodel and these are presented in Table 3.

Fuel utilization factor	UF	0.85
Operating temperature	T_{SOFC}	800°C
Anode pressure loss	Δp_a	5 mbar
Cathode pressure loss	Δp_c	10 mbar
Current density	i	300 mA cm ⁻²

Table 3: Inputs to the SOFC submodel

In the submodel only H₂ is electrochemically converted in the SOFC anode, but the model takes into account that CO produces an extra H₂ through the water-gas-shift (WGS) reaction, while four additional H₂ molecules are produced from CH₄ through internal steam reforming and WGS of produced CO (full conversion is assumed). The total mole flow of H₂ on the anode after internal steam reforming and WGS is expressed in Eq. (1).

$$\dot{n}_{H_2, tot} = \dot{n}_{H_2, in} + \dot{n}_{CO, in} + 4\dot{n}_{CH_4, in} \quad (1)$$



The amount of hydrogen that is converted depends on the fuel utilization factor (UF) and this amount is electrochemically converted in the anode. The electrode reactions and the overall fuel cell reaction are as shown in Eq. (2) to (4).

From the overall fuel cell reaction it is seen that the amount of consumed oxygen is half the amount of consumed hydrogen. The cathode outlet composition can then be found by

the following equations if the only species taking into account are O₂, N₂, CO₂, H₂O and Ar.

$$\dot{n}_{O_2,con} = \frac{UF\dot{n}_{H_2,in}}{2} \quad (5)$$

$$\dot{n}_{c,out} = \dot{n}_{c,in} - \dot{n}_{O_2,con} \quad (6)$$

$$y_{O_2,out} = \frac{\dot{n}_{c,in}y_{O_2,in} - \dot{n}_{O_2,con}}{\dot{n}_{c,out}} \quad (7)$$

$$y_{j,out} = \frac{\dot{n}_{c,in}y_{j,in}}{\dot{n}_{c,out}}, j = \{N_2, CO_2, H_2O\} \quad (8)$$

$$y_{Ar,out} = 1 - y_{O_2,out} - y_{N_2,out} - y_{CO_2,out} - y_{H_2O,out} \quad (9)$$

The fuel composition leaving the anode is calculated by the Gibbs minimization method [6] as described for the gasifier submodel. Equilibrium at the anode outlet temperature and pressure is assumed for the following species: H₂, CO, CO₂, H₂O, CH₄ and N₂. The equilibrium assumption is fair since the methane content in this study is low enough for such kind of assumption to be made. The heat consumed by the endothermic internal reforming reactions is taken into account by the Gibbs minimization method. More internal reforming means more cooling of the SOFC.

The power production from the SOFC depends on the amount of chemical energy fed to the anode, the reversible efficiency (η_{rev}), the voltage efficiency (η_v) and the fuel utilization factor (UF). It is defined in mathematical form in Eq. (10).

$$P_{SOFC} = [LHV_{H_2}\dot{n}_{H_2,in} + LHV_{CO}\dot{n}_{CO,in} + LHV_{CH_4}\dot{n}_{CH_4,in}] \eta_{rev} \eta_v UF \quad (10)$$

The reversible efficiency is the maximum possible efficiency defined as the relationship between the maximum electrical energy available (change in Gibbs free energy) and the fuels LHV. This is shown in Eq. (11) and the definition of the change in Gibbs free energy is shown in Eq. (12). The voltage efficiency express the electrochemical performance of the SOFC and the calculation of the voltage efficiency is described in the following subsection.

$$\eta_{rev} = \frac{(A\bar{g}_f)_{fuel}}{LHV_{fuel}} \quad (11)$$

$$\begin{aligned} (A\bar{g}_f)_{fuel} = & [(\bar{g}_f)_{H_2O} - (\bar{g}_f)_{H_2} - \frac{1}{2}(\bar{g}_f)_{O_2}] y_{H_2,in} \\ & + [(\bar{g}_f)_{CO_2} - (\bar{g}_f)_{CO} - \frac{1}{2}(\bar{g}_f)_{O_2}] y_{CO,in} \\ & + [(\bar{g}_f)_{CO_2} + 2(\bar{g}_f)_{H_2O} - (\bar{g}_f)_{CH_4} - 2(\bar{g}_f)_{O_2}] y_{CH_4,in} \end{aligned} \quad (12)$$

4.1 Electrochemical model

The electrochemical model is used to calculate the cell potential and the voltage efficiency of the SOFC. Both depend on the operating conditions such as temperature, pressure, gas compositions, fuel utilization and load (current density). The cell potential and voltage efficiency is defined in Eq. (13) and (14), respectively.

$$V_{cell} = E - V_{act} - V_{ohm} \quad (13)$$

$$\eta_v = \frac{V_{cell}}{E} \quad (14)$$

In the following the reversible open circuit voltage (E), the activation overpotential (V_{act}) and the ohmic overpotential (V_{ohm}) are calculated. Traditionally a concentration overpotential term is included in Eq. (13). The concentration overpotential is a result of the limitations of transporting the reactants to the active cell area. In Larminie et al. [7] it is described as a voltage drop caused by the pressure change associated with the consumption of reactants. As a result of the current being drawn from the cell, the average partial pressure of reactants is lower than at the inlet. Thus, in this study the concentration overvoltage is taken into account by using average partial pressures when calculating E and V_{act} .

E can be calculated from the Nernst equation:

$$E = \frac{-\Delta \bar{g}_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{\bar{p}_{\text{H}_2, \text{tot}} \sqrt{\bar{p}_{\text{O}_2}}}{\bar{p}_{\text{H}_2\text{O}}} \right) \quad (15)$$

Since it is assumed that all CO and CH₄ are converted to H₂ before the electrochemical reactions take place, the change in standard Gibbs free energy ($\Delta \bar{g}_f^0$) is and the number of electrons transferred for each molecule of fuel (n_e) are determined for the reaction of H₂ only. Thus, $n_e = 2$ and $\Delta \bar{g}_f^0 = (\bar{g}_f^0)_{\text{H}_2\text{O}} - (\bar{g}_f^0)_{\text{H}_2} - \frac{1}{2} (\bar{g}_f^0)_{\text{O}_2}$. The partial pressure of species j is an average across the respective electrode and is here defined as an arithmetic mean between inlet and outlet as shown in Eq. (16) and (17). The average partial pressure of available hydrogen after internal steam reforming and WGS of CH₄ and CO can be determined from the overall steam reforming and WGS reaction including all species. It is defined in Eq. (18).

$$\bar{p}_j = \left(\frac{y_{j, \text{out}} - y_{j, \text{in}}}{2} \right) p_a, \quad j = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2\} \quad (16)$$

$$\bar{p}_{\text{O}_2} = \left(\frac{y_{\text{O}_2, \text{out}} - y_{\text{O}_2, \text{in}}}{2} \right) p_c \quad (17)$$

$$\bar{p}_{\text{H}_2, \text{tot}} = \left(\frac{\bar{p}_{\text{H}_2} + \bar{p}_{\text{CO}} + 4\bar{p}_{\text{CH}_4}}{\bar{p}_{\text{H}_2} + \bar{p}_{\text{CO}} + 3\bar{p}_{\text{CH}_4} + \bar{p}_{\text{CO}_2} + \bar{p}_{\text{H}_2\text{O}} + \bar{p}_{\text{N}_2}} \right) p_a \quad (18)$$

The activation overpotential is due to an energy barrier (activation energy) that the reactants must overcome in order to drive the electrochemical reactions. The activation overpotential is non-linear and is dominant at low current densities (i). The activation overpotential is defined as (cf. [8]):

$$V_{\text{act}} = V_{\text{act}, a} + V_{\text{act}, c} = \frac{2RT}{n_e F} \left[\sinh^{-1} \left(\frac{i + i_n}{2i_{0, a}} \right) + \sinh^{-1} \left(\frac{i + i_n}{2i_{0, c}} \right) \right] \quad (19)$$

The internal current density (i_n) is added to the actual fuel cell current density in order to account for the mixed potential caused by fuel crossover. The importance of the internal current density in the case of SOFCs is much less than for low temperature fuel cells and the value of i_n is usually very small [7]. The exchange current density (i_0) is a measure of the level of activity on the electrode at $i=0$ mA cm⁻² and is defined as (cf. [9]):

$$i_{0, a} = 2.13 \times 10^7 \left(\frac{\bar{p}_{\text{H}_2, \text{tot}} \bar{p}_{\text{H}_2\text{O}}}{p_a^2} \right) \exp \left(\frac{-110000}{RT} \right) \quad (20)$$

$$i_{0, c} = 1.49 \times 10^7 \left(\frac{\bar{p}_{\text{O}_2}}{p_c} \right)^{0.25} \exp \left(\frac{-110000}{RT} \right) \quad (21)$$

The ohmic overpotential is caused by the electrical resistance for the ions passing through the electrolyte as well as for the electrons passing through the electrodes and interconnects. The ohmic overpotential is defined below (cf. [9] and [12]).

$$V_{\text{ohm}} = i ASR \quad (22)$$

$$ASR = ASR_a + ASR_c + ASR_e + ASR_i \quad (23)$$

$$ASR_j = \delta_j a_{\text{ohm},j} \exp\left(\frac{b_{\text{ohm},j}}{T}\right), j = \{a, c, e, i\} \quad (24)$$

The thicknesses of the different layers (δ) and the constants a_{ohm} and b_{ohm} used are listed in Table 4.

R	$8.314 \text{ J K}^{-1} \text{ mol}^{-1}$
F	96485 C mol^{-1}
n_e	2
i_n	2 mA cm^{-2} [9]
δ_a	$750 \times 10^{-4} \text{ cm}$ [10]
δ_c	$50 \times 10^{-4} \text{ cm}$ [10]
δ_e	$40 \times 10^{-4} \text{ cm}$ [10]
δ_i	$100 \times 10^{-4} \text{ cm}$ [11]
$a_{\text{ohm},a}$	$0.00298 \times 10^{-3} \text{ k}\Omega\text{cm}$ [12]
$b_{\text{ohm},a}$	-1392 K [12]
$a_{\text{ohm},c}$	$0.00811 \times 10^{-3} \text{ k}\Omega\text{cm}$ [12]
$b_{\text{ohm},c}$	600 K [12]
$a_{\text{ohm},e}$	$0.00294 \times 10^{-3} \text{ k}\Omega\text{cm}$ [12]
$b_{\text{ohm},e}$	10350 K [12]
$a_{\text{ohm},i}$	$0.1256 \times 10^{-3} \text{ k}\Omega\text{cm}$ [12]
$b_{\text{ohm},i}$	4690 K [12]

Table 4: Inputs for the electrochemical model

4.2 Electrochemical model calibration

The described electrochemical model has been calibrated against experimental data, see Figure 2.

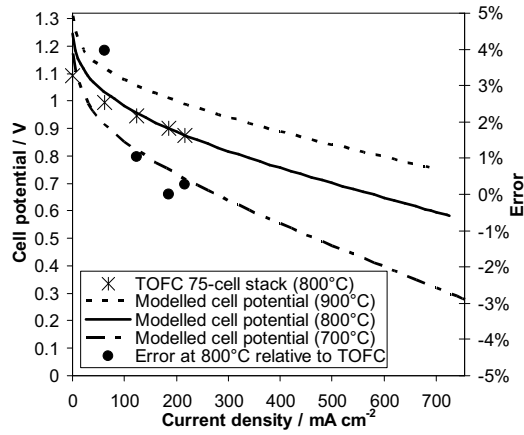


Figure 2: Single cell polarization curves based on a 75-cell stack and the SOFC model, respectively

Since the model aims at the performance of 2nd generation SOFCs from Topsoe Fuel Cell A/S (TOFC) and Risø National Laboratory, published data for this SOFC type has been used. The ASR has been calibrated against a value of $0.15 \Omega \text{ cm}^2$ at 850°C as published by [13] and the resulting cell potential has been calibrated against a polarization curve

(75-cell stack, $12 \times 12 \text{ cm}^2$, 800°C and fuelled with H_2 and N_2) published by [14]. An active cell area of 81 cm^2 has been assumed. Both modelled and experimental data as well as the error relative to the experimental data are presented in Figure 2.

The model shows excellent agreement with the experimental data above a current density of 100 mA cm^{-2} . The current density of 300 mA cm^{-2} is chosen to represent the SOFC load in the following results.

5 Peripheral equipment

Modelling of peripheral components like compressors, turbines and heat exchangers are standard and therefore not described in detail.

The throughput of wet biomass is 154.8 kg h^{-1} (corresponds to $499.2 \text{ kW}_{\text{th}}$ (LHV)). Thus it is assumed that the Viking gasifier can be scaled up from a nominal $\sim 75 \text{ kW}_{\text{th}}$ [3]. The biomass dryer reduces the water content in the biomass from 32.2 wt-% to 5 wt-% by heating it to 150°C and the air for the gasifier is preheated to 780°C by the hot product gas.

The inlet temperature to the SOFC anode and cathode are maintained at 150°C and 200°C below the outlet temperature, respectively.

The pressure loss in every component in the SOFC air supply stream and burner exhaust stream is assumed to be 10 mbar, while the pressure loss in each of the rest of the components is assumed to be 5 mbar, except the burner that has a pressure loss of 0.6% (equals 1.5 mbar when 2.5 bar at inlet).

The gas cleaner is a baghouse filter removing particulates and it is assumed that the cleaned syngas can be used directly in a SOFC. The condenser removes some of the water content in the syngas resulting in a content of water in the cleaned and dried syngas of 12.7 vol-%. The resulting steam to carbon ratio (S/C) is 0.41, which is somewhat low, but is justified by the very low tar content in the Viking syngas.

The isentropic and mechanical efficiency of the compressors are 75% and 98%, respectively, and the isentropic efficiency of the MGT expander is 84%. The performance of the compressors and the MGT expander are taken from Fryda et al. [2] and corresponds to common performance data for a MGT of this scale. The recuperator effectiveness is assumed to be 85% and the generator efficiency is assumed to be 99%. In the Gasifier-SOFC configuration the SOFC operating pressure is ~ 1 bar and in the Gasifier-SOFC-MGT case the SOFC operating pressure is 2.5 bar (this pressure is varied in the results section).

No heat losses are taken into account. Introducing heat losses from the gas cleaner will only affect the heat production from the condenser since the temperature after the condenser is fixed to 50°C .

The outlet pressure from the MGT depends on the total pressure loss downstream the MGT, since it is the exhaust pressure which is fixed to 1.013 bar. Because of the recuperator and exhaust cooler the outlet pressure from the MGT is 1.033 bar. The district heating (DH) water is assumed to be 30°C at inlet and 80°C at outlet.

6 Results and discussion

In the following results the inputs presented in the previous sections are used unless something else is stated. The system configurations are previously described in detail.

The performance of the different system configurations vary greatly with the operating conditions and namely the operating pressure of the SOFC (in the Gasifier-SOFC-MGT case) are of great importance to the resulting system performance. The Gasifier-SOFC-MGT configuration has an optimum with regard to its operating pressure, while the

Gasifier-SOFC arrangement always operates at atmospheric pressure – illustrated in Figure 3. The Gasifier-SOFC configuration performs an electric efficiency of 36.4%. By combining the SOFC and MGT in the Gasifier-SOFC-MGT configuration the electrical efficiency reaches 50.3% at an optimum operating pressure of 2.5 bar. This is a substantial increase in efficiency caused by the utilization of unconverted fuel from the SOFC (fuel utilization of 85%) in the MGT as well as the pressurized operation of the SOFC. In the Gasifier-SOFC-MGT case the turbine inlet temperature (TIT) is varying with the SOFC operating pressure and has a value of 697°C at 2.5 bar. It is the recuperator that ensures an optimum at a relatively low operating pressure.

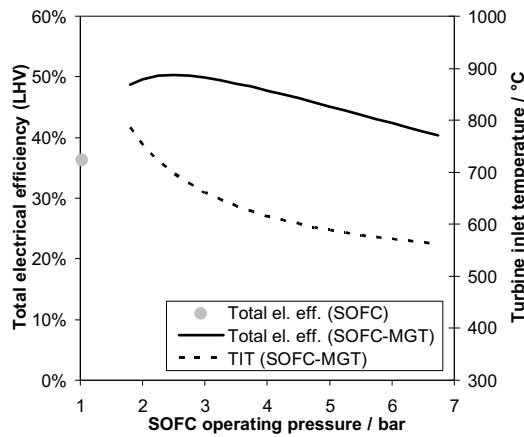


Figure 3: Electric efficiency and TIT at different SOFC operating pressures

The performance of both system arrangements strongly depend on the SOFC operating temperature as depicted in Figure 4. Decreasing the temperature by 100°C to 700°C lowers the electrical efficiency to 28.8% and 44.4% in the Gasifier-SOFC and Gasifier-SOFC-MGT case, respectively. This corresponds to a drop of 7.6 and 5.9 percentage points, respectively. The research and development working on lowering the SOFC operating temperature in order to use cheaper materials will influence the system performance presented here and potentially other bottoming cycles could be beneficial, e.g. a Rankine cycle.

The sensitivity of the model results to the chosen SOFC current density is shown in Figure 5.

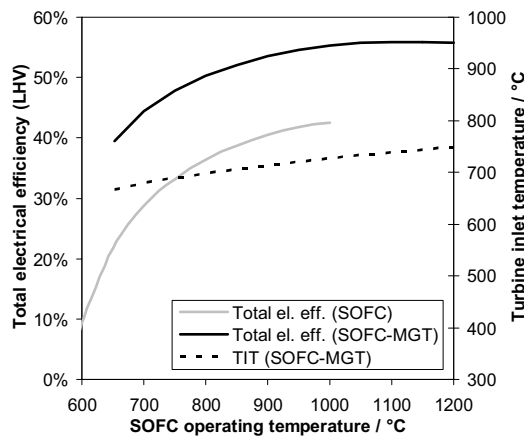


Figure 4: Electric efficiency and TIT at different SOFC operating temperatures

At the reference current density value of 300 mA cm^{-2} the SOFC voltage efficiency is 39.6% in the Gasifier-SOFC arrangement and 40.8% in the Gasifier-SOFC-MGT case. The difference is due to the pressure. Raising the SOFC load to 500 mA cm^{-2} reduces the

voltage efficiency (defined in Eq. (14)) to 34.6% and 35.7% in the Gasifier-SOFC and Gasifier-SOFC-MGT cases, respectively, meaning a reduction in the total electrical efficiency to 31.5% and 46.7% - a drop of 4.9 and 3.6 percentage points. This is a relative change in electrical efficiency of 13.5% and 7.2%, respectively, for a 66.7% increase in current density.

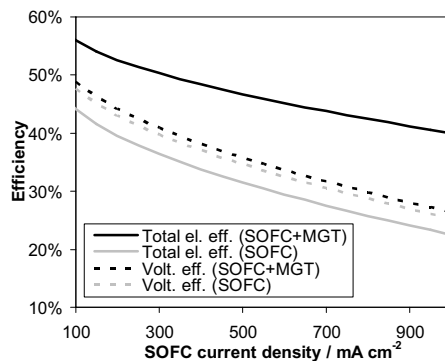


Figure 5: Electrical efficiency and SOFC voltage efficiency as a function of SOFC current density

Key data for the two system configurations studied are presented in Table 5 based on the reference input values presented in the previous sections. The Gasifier-SOFC-MGT configuration clearly has the best electrical efficiency, while the CHP efficiencies do not differ significantly. In the Gasifier-SOFC-MGT case, the power production is mainly from the SOFC producing 76.4% of the power. The exact values of the efficiencies will be slightly lower when incorporating heat losses, a more accurate efficiency of the gasifier system and possible more extensive gas cleaning, but the comparison of the systems performance is still valid.

		Gasifier -SOFC	Gasifier -SOFC-MGT
Biomass input	/ kg h ⁻¹	154.8	154.8
	/ kW _{th,LHV}	499.2	499.2
p_{SOFC} / bar		1.034	2.5
$P_{\text{MGT,net}}$ / kW _{el}		-	59.2
$P_{\text{SOFC,net}}$ / kW _{el}		181.5	191.8
$P_{\text{total,net}}$ / kW _{el}		181.5	251.0
DH production / kJ s ⁻¹		216.6	146.7
η_{el} / % (LHV)		36.4	50.3
η_{CHP} / % (LHV)		79.74	79.68

Table 5: Key data for the studied systems

7 Conclusion

A study on the system performance of an up scaled Viking gasifier (~500 kW_{th}) with either a downstream SOFC or SOFC-MGT arrangement has been conducted by zero dimensional process modelling. A SOFC submodel has been developed including an electrochemical model predicting the SOFC performance at different operating conditions. This submodel has been calibrated against published TOFC stack performance data. The reference conditions for the SOFC has been an operating temperature of 800°C, a fuel utilization of 85% and a current density of 300 mA cm⁻². The optimal operating SOFC-MGT pressure has been found to be 2.5 bar, while the SOFC without MGT operated at atmospheric pressure. The MGT utilized the unconverted syngas from the SOFC to produce more power as well as pressurizing the SOFC bettering the electrical efficiency compared to operation with the SOFC alone -

from $\eta_{el}=36.4\%$ to $\eta_{el}=50.3\%$. These efficiencies were very sensitive to the SOFC operating temperature, while only a moderate sensitivity to the SOFC current density was observed.

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Appendix J IMPROVED PREDICTION OF THE SOFC PERFORMANCE

In reality, the electrochemical performance of an SOFC is distributed over the cell area due to varying species concentrations, temperature, and pressure. Thus, making a lumped model reliable can be challenging. Nevertheless, that is a goal of this study, and in this Appendix an improved approach is presented. The improved model is developed after generating the results presented in this thesis.

Eq. (4.23) in the presented SOFC component model assumes that the average partial pressure of hydrogen used to predict the electrochemical performance of the SOFC is the sum of average partial pressure of H_2 , CO , and four times CH_4 in the anode compartment due to the steam reforming and water-gas-shift reactions. By using this equivalent hydrogen partial pressure in the presented Nernst equation (eq. (4.24)), the influence of species like CO_2 is neglected. This might be valid in water-rich environments without CO_2 , but with substantial amounts of CO_2 present, the balance between reactants and products in the Nernst equation will be off target. Thus, a better way of predicting the average species concentrations and the corresponding electrochemical performance of the SOFC is presented in this Appendix together with estimates on the influence of using the original SOFC model instead of the approach presented here.

Improved Approach

In the improved approach, the partial pressures of all anode species are determined by averaging between the chemical equilibrium composition at the inlet conditions and the chemical equilibrium composition at the outlet conditions, eq. (J.1). Chemical equilibrium at both inlet and outlet are based on

the SOFC operating pressure and the temperature of the solid structure of the SOFC (i.e., the SOFC operating temperature). The only difference between the inlet and outlet is the addition of oxygen from the cathode side prior to the outlet. Assuming chemical equilibrium at the anode inlet is fair because the high-temperature and active catalyst containing anode environment ensures fast steam reforming and WGS to reach equilibrium [17]. In the approach presented in Chapter 4, the inlet composition is not at chemical equilibrium, but instead the anode fuel feed composition is directly used. By applying Gibbs free energy minimization at the anode inlet, the gas composition is ensured to be at chemical equilibrium in the improved approach.

$$\bar{p}_j = \left(\frac{y_{j,\text{out,eq}} + y_{j,\text{in,eq}}}{2} \right) \bar{p}_a, j = \{\text{H}_2, \text{CO}, \text{CH}_4, \text{CO}_2, \text{H}_2\text{O}, \text{N}_2\} \quad (\text{J.1})$$

Furthermore, the Nernst potential is determined at both inlet and outlet. An arithmetic mean between the inlet Nernst potential and the outlet Nernst potential is chosen to represent the average Nernst potential of the cell (eqs. (J.2) to (J.4)). The actual Nernst potential is distributed across the cell area and could be determined more precisely by integrating over the cell length or area, but in a lumped model that is not possible, thus averaging between inlet and outlet is used as an estimate.

$$E_{\text{in}} = \frac{-\Delta g_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{p_{\text{H}_2,\text{in,eq}} \sqrt{p_{\text{O}_2,\text{in}}}}{p_{\text{H}_2\text{O},\text{in,eq}}} \right) \quad (\text{J.2})$$

$$E_{\text{out}} = \frac{-\Delta g_f^0}{n_e F} + \frac{RT}{n_e F} \ln \left(\frac{p_{\text{H}_2,\text{out,eq}} \sqrt{p_{\text{O}_2,\text{out}}}}{p_{\text{H}_2\text{O},\text{out,eq}}} \right) \quad (\text{J.3})$$

$$\bar{E} = \frac{E_{\text{in}} + E_{\text{out}}}{2} \quad (\text{J.4})$$

The equations presented above should replace eqs. (4.21), (4.23), and (4.24). By means of this improved alternative, the estimation of the Nernst potential and SOFC performance is valid for a variety of fuel compositions including CO₂-rich mixtures. The improved SOFC model is calibrated in the same way and against the same experimental data as described in Section 4.1.1. By performing the same calibration, the SOFC performance will be similar at the operating conditions of experimental data used for calibration. Since the operating conditions of the SOFC in the studied plant designs are different from the experimental data, the changes in the model will still affect the

SOFC performance in the plant studies and the consequences are estimated and discussed below.

Consequences

The results presented in Chapter 4, Chapter 6, and Chapter 7 will change when applying the suggested improvements above, because the electrical efficiency of the SOFC will be different at the same operating conditions. Instead of recalculating all the results in these Chapters, this Section will deal with how much the operating conditions of the SOFC should be modified to reach similar SOFC performance as in the original results. Several of the operating conditions of the SOFC (e.g., current density and operating temperature) are arbitrary chosen within realistic operational range, thus variation of some of these conditions will not make the results less reliable, and the comparison of conceptual plant designs and the system-level optimization will still be valid.

In Table J.1, the operational data for the SOFC model is presented using the original and improved approaches. It is clear that the SOFC performance is lower in the improved SOFC model at the same operating conditions, and this is mainly due to an increased area specific resistance (*ASR*). *ASR* includes all overpotentials and is defined as follows:

$$ASR = \frac{E - V_{\text{cell}}}{i} \quad (\text{J.5})$$

Table J.1: Data from original and improved SOFC model using product gas.

	Original SOFC model	Improved SOFC model
$p_{\text{SOFC}} / \text{bar}$	2.5	2.5
$T_{\text{SOFC}} / ^\circ\text{C}$	800	800
$i / \text{mA cm}^{-2}$	300	300
E / V	0.965	0.925
$V_{\text{cell}} / \text{V}$	0.820	0.661
$ASR / \Omega \text{ cm}^2$	0.486	0.880
$\eta_v / \%$	84.9	71.5
$\eta_{\text{rev}} / \%$	70.3	68.8
$U_F / \%$	85.0	85.0
$\eta_{\text{SOFC}} / \%$	50.7	41.8

By use of the improved model, the average partial pressure of hydrogen will be lower than in the original model (because eq. (4.23) is neglected). The Nernst potential drops 40 mV (cf., Table J.1), but also the *ASR* is affected because of its dependence on the partial pressures. The *ASR* increases

mainly because of the expression describing the anodic exchange current density in eq. (4.28), in which CO is considered inert in the modified model and a fuel on equal terms as H₂ in the original model. In reality, CO is neither inert or can be considered on equal terms as H₂ (due to reduced reaction rate), thus the improved model can be seen as a worst case scenario and the original model as a best case scenario. The truth will be somewhere in between.

By changing the operating temperature and current density, the SOFC performance can be adjusted to meet the original SOFC model. This is illustrated in Table J.2, where first the current density, then the operating temperature, and finally both are adjusted.

Table J.2: Data from improved and adjusted SOFC model.

	Improved SOFC model		
	adjusted i	adjusted T_{SOFC}	adjusted i and T_{SOFC}
$p_{\text{SOFC}} / \text{bar}$	2.5	2.5	2.5
$T_{\text{SOFC}} / ^\circ\text{C}$	800	950	875
$i / \text{mA cm}^{-2}$	130	300	225
E / V	0.925	0.863	0.894
$V_{\text{cell}} / \text{V}$	0.801	0.778	0.788
$ASR / \Omega \text{ cm}^2$	0.947	0.285	0.472
$\eta_v / \%$	86.7	90.1	88.1
$\eta_{\text{rev}} / \%$	68.8	63.7	66.2
$U_F / \%$	85.0	85.0	85.0
$\eta_{\text{SOFC}} / \%$	50.7	48.8	49.6

When adjusting either the current density or the SOFC temperature individually to meet similar η_{SOFC} as in the original SOFC model, the resulting ASR is still different from the one found in the original model. By adjusting both current density and temperature, similar η_{SOFC} and ASR can be obtained. The problem of changing the operating temperature of the SOFC is that it will affect the surrounding system when incorporated into a plant. Therefore it can be concluded that for the original results to be valid for both SOFC component and plant designs, the current density should be lowered to 130 mA cm⁻² when using the improved SOFC modelling approach. In other words, the original results correspond to an SOFC performance at 130 mA cm⁻² when using the improved approach. This is a low current density compared to typical operation between 200 and 300 mA cm⁻², but when noting that the experimental data used for calibration is based on an SOFC from around year 2005, recent and future development will ensure a similar SOFC performance at a higher and more typical load.

Using the improved and current density-adjusted SOFC component model in the plant simulations, the plant performance results in Table J.3 are obtained. No decisive changes in the overall performances are seen. The lower current density (load) means that the SOFC stack size should increase for the plant to produce the same electric power, though. This will also influence the economic aspects of the plant in a negative manner.

Table J.3: Plant performance data using improved and adjusted SOFC model (values in brackets are the original data from Table 6.1 and Table 7.2).

	Plant configuration		
	SOFC	SOFC-MGT	Optimized SOFC-MGT
$i / \text{mA cm}^{-2}$	130 (300)	130 (300)	130 (300)
$T_{\text{SOFC}} / ^\circ\text{C}$	800 (800)	800 (800)	800 (800)
Optimal $PR / -$	~ 1 (~ 1)	2.5 (2.5)	2.7 (2.7)
$V_{\text{cell}} / \text{V}$	0.782 (0.800)	0.801 (0.820)	0.803 (0.822)
$\eta_{\text{el, total system}} / \%$ (LHV)	43.9 (43.1)	55.7 (55.0)	58.8 (58.2)

If the improved SOFC model were to be used without the adjustments, the plant performances would decrease as shown in Table J.4. As discussed above, the original data (in brackets) represents a best case scenario and the new data represents a worst case scenario.

Table J.4: Plant performance data using improved and unadjusted SOFC model (values in brackets are the original data from Table 6.1 and Table 7.2).

	Plant configuration		
	SOFC	SOFC-MGT	Optimized SOFC-MGT
$i / \text{mA cm}^{-2}$	300 (300)	300 (300)	300 (300)
$T_{\text{SOFC}} / ^\circ\text{C}$	800 (800)	800 (800)	800 (800)
Optimal $PR / -$	~ 1 (~ 1)	2.5 (2.5)	2.6 (2.7)
$V_{\text{cell}} / \text{V}$	0.641 (0.800)	0.661 (0.820)	0.662 (0.822)
$\eta_{\text{el, total system}} / \%$ (LHV)	35.6 (43.1)	49.5 (55.0)	52.7 (58.2)

Suggestion for Further Improvement

The improved approach presented in this Appendix could be further improved, but that is outside the work of this project. The estimation of the Nernst potential is satisfactory, but the ASR is overestimated when CO is considered inert. On the other hand, CO cannot be considered equal to H_2 . It is suggested to investigate alternative expressions for the anodic exchange current density, and the following approach is specifically suggested; (1) find separate anodic exchange current density expressions for H_2 – H_2O and

CO–CO₂ environments, (2) calculate the anodic exchange current density for H₂–H₂O and CO–CO₂ at both anode inlet and outlet and determine the average between inlet and outlet of H₂–H₂O and CO–CO₂, respectively, and (3) weigh the two average anodic exchange current densities by the concentrations of H₂ and CO in the anode compartment to determine an overall anodic exchange current density. In this manner, the evaluation of the activation overpotential will be more generic, and the SOFC and plant performances will be in between the best and worst case scenarios presented above.

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